# A study on quantum gases: bosons in optical lattices and the one-dimensional interacting Bose gas

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# Summary


## Bosons in optical lattices

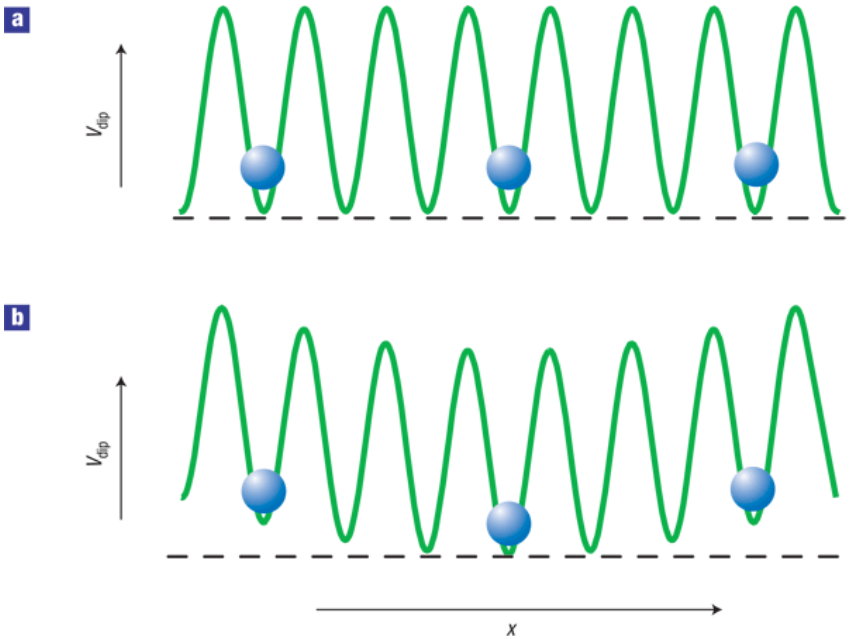
- Mott-insulator-superfluid quantum phase transition
- The zero-temperature regime
- The system at finite temperature

## One-dimensional interacting Bose gas

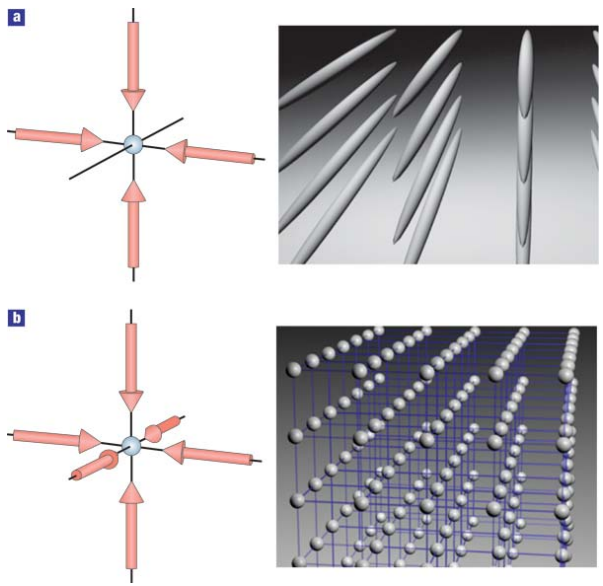
- Asymptotic behavior of the momentum distribution
- The Tonks-Girardeau limit
- Scaling properties
  - Zero-temperature scaling
  - Large-temperature scaling
  - Generalized scaling conjecture

# Optical lattices

- Optical lattices: Trapping of atoms due to the interaction between the laser-generated electric field and the atomic electric dipole.




- Optical lattices provide an easily and fully controllable environment for the study of BEC and cold atoms in general.




I. Bloch, *Nature Physics* **1**, 23 (2005)

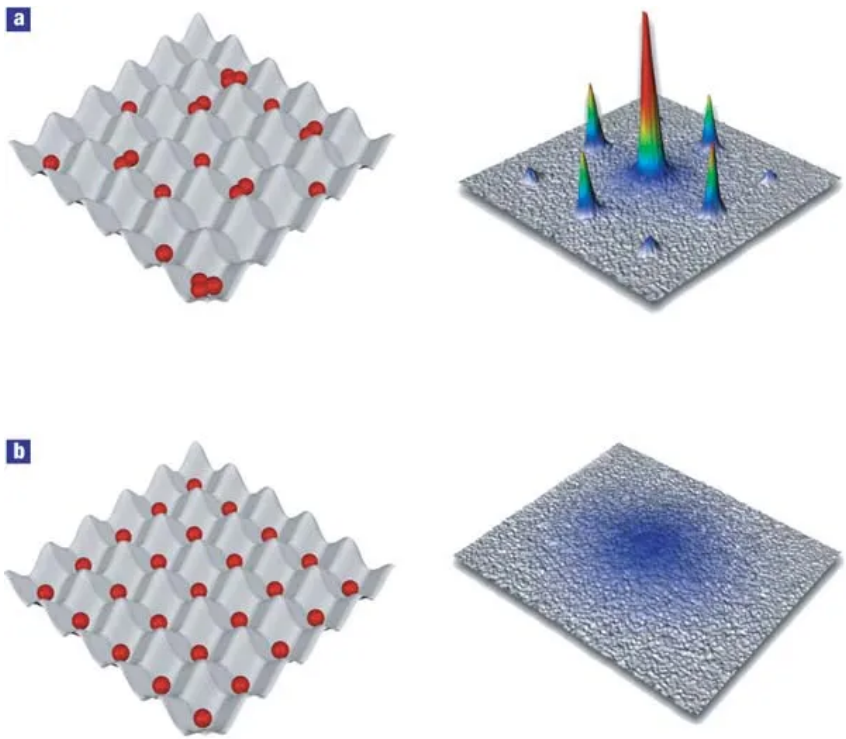
# The Bose-Hubbard model

Bose-Hubbard Hamiltonian for spinless bosonic atoms confined in an optical lattice:

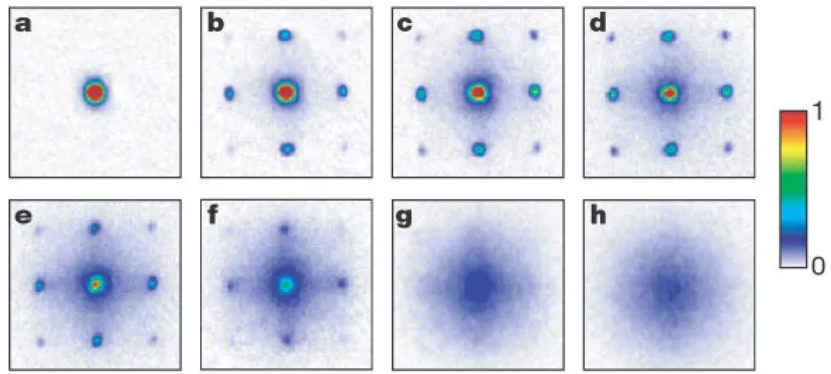
$$\hat{H}_{BH} = \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i - J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j - \mu \sum_i \hat{a}_i^\dagger \hat{a}_i. \tag{1}$$

- $U$ stands for the on-site interaction parameter describing the interaction between particles.
- $J$ represents the hopping parameter.
- $\langle i, j \rangle$ represents a restriction: only nearest neighbors transitions are considered.
- $\mu$ denotes the chemical potential.

# Phase transition




I. Bloch, *Nature Physics* **1**, 23 (2005)




M. Greiner *et al.*, *Nature* **415**, 39 (2002)

(a) If $J \gg U$, the system is in the superfluid phase: the picture in the momentum space presents some peaks which represent the atoms sharing the respective momentum.
(b) If $U \gg J$, the system is in the Mott insulator phase: the atoms are localized in its respective potential minima with low momentum.

# Mean-field approximation

From the Bose-Hubbard Hamiltonian

$$\hat{H}_{BH} = \frac{U}{2}\sum_i \left(\hat{n}_i^2 - \hat{n}_i\right) - \mu\sum_i \hat{n}_i - J\sum_{\langle i,j\rangle} \hat{a}_i^\dagger \hat{a}_j, \tag{2}$$

we take the following steps:

1. Perform the substitution $\hat{a}_i = \Psi + \delta\hat{a}_i$ and $\hat{a}_i^\dagger = \Psi^* + \delta\hat{a}_i^\dagger$, where $\Psi$ is called *mean-field*;
2. Neglect quadratic terms of fluctuation, $\delta^2$.

Such steps lead to the mean-field Hamiltonian,

$$\hat{H}_{MF} = \frac{U}{2}\sum_i \left(\hat{n}_i^2 - \hat{n}_i\right) - \sum_i \mu\hat{n}_i - Jz\sum_i \left(\Psi^*\hat{a}_i + \Psi\hat{a}_i^\dagger - \Psi^*\Psi\right). \tag{3}$$

As $\hat{H}_{MF}$ is a local Hamiltonian, we can restrict ourselves to one lattice site Hamiltonian

$$\hat{H} = \frac{U}{2}\left(\hat{n}^2 - \hat{n}\right) - \mu\hat{n} - Jz\left(\Psi^*\hat{a} + \Psi\hat{a}^\dagger - \Psi^*\Psi\right). \tag{4}$$

# Landau theory

- Landau expansion for the energy in the vicinity of the phase transition

$$\mathcal{F} = a_0 + a_2|\Psi|^2 + a_4|\Psi|^4 + \cdots . \tag{5}$$

- Extremizing it with respect to the order parameter

$$\frac{\partial \mathcal{F}}{\partial \Psi} = \Psi^* \left(a_2 + 2a_4|\Psi|^2\right) = 0, \tag{6}$$

the solutions are

$$\Psi = 0, \quad \text{(Mott insulator)} \tag{7a}$$

$$|\Psi|^2 = -\frac{a_2}{2a_4}. \quad \text{(Superfluid)} \tag{7b}$$

- The phase boundary is given by $a_2 = 0$.

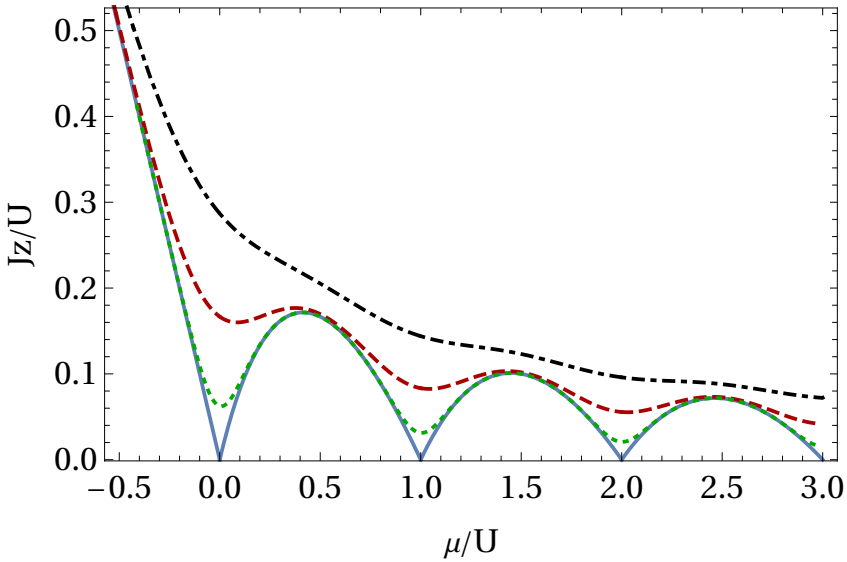
# Phase diagram

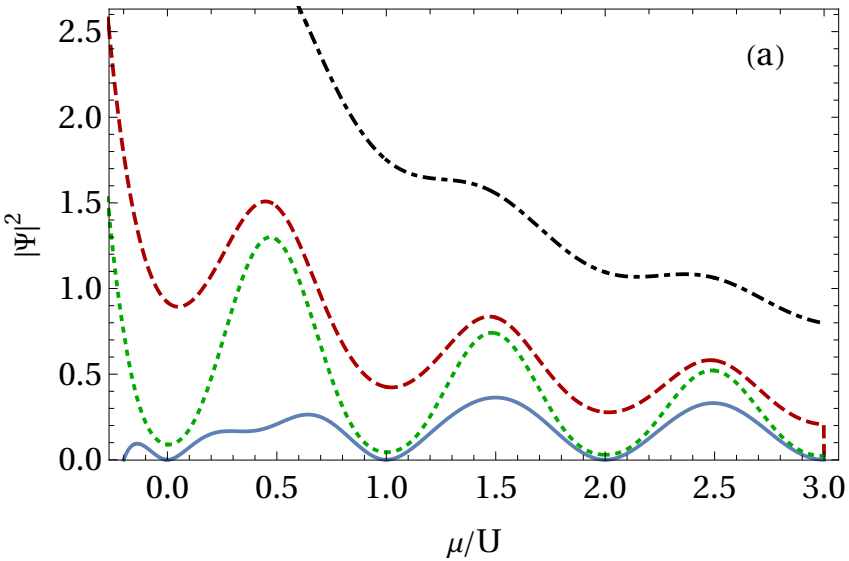
- Phase boundary:

$$a_2 = 0. \qquad (8)$$

- Condensate density:

$$|\Psi|^2 = -\frac{a_2}{2a_4}. \qquad (9)$$




F. T. Sant'Ana *et al.*, *Phys. Rev. A* **100** 043609 (2019)

- The order parameter depicts a nonphysical behavior: it vanishes where no phase transition occurs!

# Degeneracies

- The reason for the vanishing of the condensate density in a region of the phase diagram where there is no phase transition are the degeneracies that occur between two consecutive Mott lobes:

$$\begin{aligned} E_n &= E_{n+1} \\ \frac{U}{2} n(n-1) - \mu n &= \frac{U}{2} n(n+1) - \mu(n+1) \\ \frac{\mu}{U} &= n \end{aligned} \tag{10}$$

- Proposal: to develop a method for calculating physical quantites for the zero- and finite-temperature systems taking into account the degeneracies.

# The zero-temperature regime

PHYSICAL REVIEW A **99**, 063603 (2019)

## Improving mean-field theory for bosons in optical lattices via degenerate perturbation theory

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The objective of this paper is the theoretical description of the Mott insulator to superfluid quantum phase transition of a Bose gas in an optical lattice. In former works the Rayleigh-Schrödinger perturbation theory was used within a mean-field approach, which yields partially nonphysical results since the degeneracy between two adjacent Mott lobes is not taken into account. In order to correct such nonphysical results we apply the Brillouin-Wigner perturbation theory to the mean-field approximation of the Bose-Hubbard model. Detailed explanations of how to use the Brillouin-Wigner theory are presented, including a graphical approach that allows one to efficiently keep track of the respective analytic terms. To prove the validity of this computation, the results are compared with other works. Besides the analytic calculation of the phase boundary from Mott insulator to superfluid phase, the condensate density is also determined by simultaneously solving two algebraic equations. The analytical and numerical results turn out to be physically meaningful and can cover a region of system parameters inaccessible until now. Our results are of particular interest provided a harmonic trap is added to the former calculations in a homogeneous system, in view of describing an experiment within the local-density approximation. Thus, the paper represents an essential preparatory work for determining the experimentally observed wedding cake structure of particle-density profile at both finite temperature and finite hopping.

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# The zero-temperature regime: a Brillouin-Wigner perturbation theory treatment

The BWPT amounts to derive an effective Hamiltonian for an arbitrarily chosen Hilbert subspace:

- Let $\mathcal{P}$ and $\mathcal{Q}$ be two complementary Hilbert subspaces, whose projection operators satisfy

$$\hat{\mathcal{P}} + \hat{\mathcal{Q}} = \hat{\mathbb{1}}. \tag{11}$$

- Reformulating the time-independent Schrödinger equation $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$ as

$$\hat{\mathcal{P}}\left[\hat{H} + \lambda\hat{V}\hat{\mathcal{Q}}\left(E_n - \hat{\mathcal{Q}}\hat{H}\hat{\mathcal{Q}}\right)^{-1}\hat{\mathcal{Q}}\lambda\hat{V}\right]\hat{\mathcal{P}}|\Psi_n\rangle = E_n\hat{\mathcal{P}}|\Psi_n\rangle, \tag{12}$$

which represents a single equation for $\hat{\mathcal{P}}|\Psi_n\rangle$.

# Brillouin-Wigner perturbation theory

- The resulting equation for $\hat{\mathcal{P}}|\Psi_n\rangle$ is of the form of a time-independent Schrödinger equation

$$\hat{\mathcal{P}}\hat{H}_{\text{eff}}\hat{P}|\Psi_n\rangle = E_n\hat{\mathcal{P}}|\Psi_n\rangle, \tag{13}$$

with

$$\hat{H}_{\text{eff}} \equiv \hat{H} + \lambda^2\hat{V}\hat{\mathcal{Q}}\left(E_n - \hat{\mathcal{Q}}\hat{H}\hat{\mathcal{Q}}\right)^{-1}\hat{\mathcal{Q}}\hat{V}. \tag{14}$$

- The effective Hamiltonian can then be expanded in series with respect to $\lambda$:

$$\begin{aligned}\hat{H}_{\text{eff}} =& \hat{H}_0 + \lambda\hat{V} + \lambda^2\sum_{I\in\mathcal{Q}}\frac{\hat{V}|\Psi_I^{(0)}\rangle\langle\Psi_I^{(0)}|\hat{V}}{E_n - E_I^{(0)}} \\ &+ \lambda^3\sum_{I,I'\in\mathcal{Q}}\frac{\hat{V}|\Psi_I^{(0)}\rangle\langle\Psi_I^{(0)}|\hat{V}|\Psi_{I'}^{(0)}\rangle\langle\Psi_{I'}^{(0)}|\hat{V}}{\left(E_n - E_I^{(0)}\right)\left(E_n - E_{I'}^{(0)}\right)} \\ &+ \lambda^4\sum_{I,I',I''\in\mathcal{Q}}\frac{\hat{V}|\Psi_I^{(0)}\rangle\langle\Psi_I^{(0)}|\hat{V}|\Psi_{I'}^{(0)}\rangle\langle\Psi_{I'}^{(0)}|\hat{V}|\Psi_{I''}^{(0)}\rangle\langle\Psi_{I''}^{(0)}|\hat{V}}{\left(E_n - E_I^{(0)}\right)\left(E_n - E_{I'}^{(0)}\right)\left(E_n - E_{I''}^{(0)}\right)} \\ &+ \cdots.\end{aligned} \tag{15}$$

# One-state approach

- Let $\hat{\mathcal{P}}$ be composed of one state:

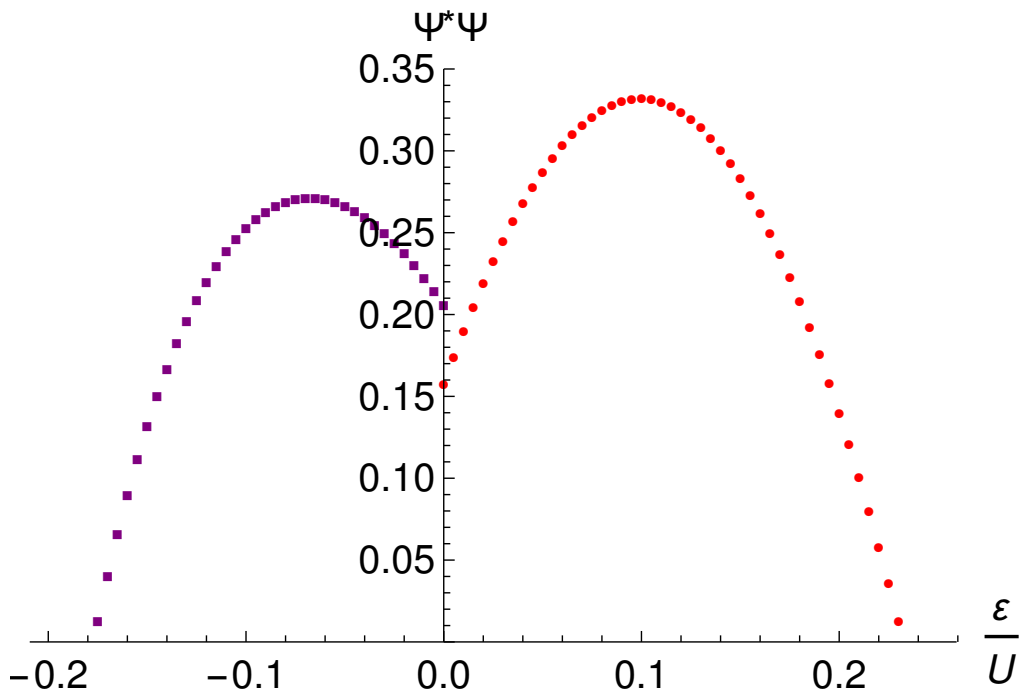
$$\hat{\mathcal{P}} = |n\rangle\langle n|. \tag{16}$$

- Then, the ground state energy, $E_n = \langle \Psi_n^{(0)} | \hat{H}_{\text{eff}} | \Psi_n^{(0)} \rangle$, is given by

$$\begin{aligned} E_n =& E_n^{(0)} + \lambda J z \Psi^* \Psi + \lambda^2 J^2 z^2 \Psi^* \Psi \left( \frac{n}{E_n - E_{n-1}^{(0)}} + \frac{n+1}{E_n - E_{n+1}^{(0)}} \right) \\ &+ \lambda^3 J^3 z^3 \left(\Psi^* \Psi\right)^2 \left[ \frac{n}{\left(E_n - E_{n-1}^{(0)}\right)^2} + \frac{n+1}{\left(E_n - E_{n+1}^{(0)}\right)^2} \right] + \cdots . \end{aligned} \tag{17}$$

# Condensate density

- The condensate density can be calculated by iteratively solving Eq. (17) together with $\partial E_n / (\Psi \partial \Psi^*) = 0$.




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# Two-state approach

- Let $\hat{\mathcal{P}}$ be composed of two states:

$$\hat{\mathcal{P}} = |n\rangle\langle n| + |n+1\rangle\langle n+1|. \tag{18}$$

- Now we have a determinantal equation for the energy

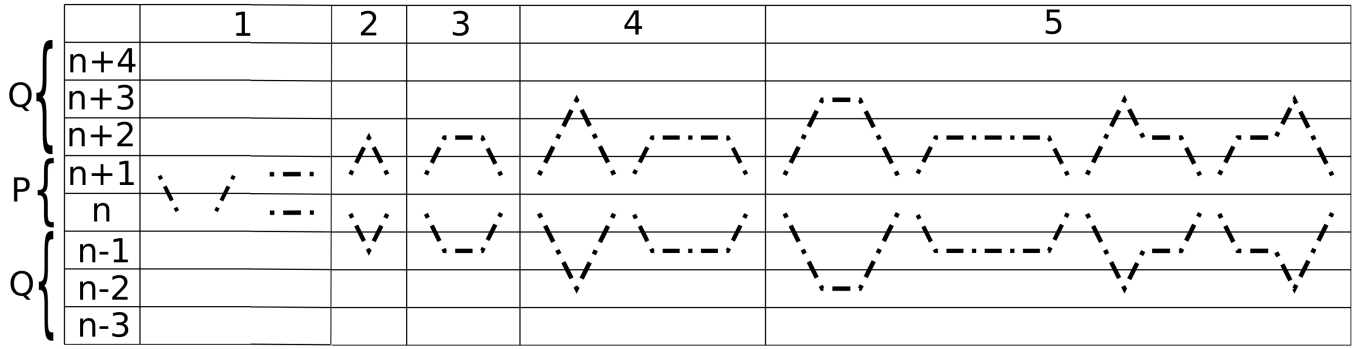
$$\begin{vmatrix} H_{\mathrm{eff},n,n} - E_n & H_{\mathrm{eff},n,n+1} \\ H_{\mathrm{eff},n+1,n} & H_{\mathrm{eff},n+1,n+1} - E_n \end{vmatrix} = 0. \tag{19}$$

- We can extract physical quantites from

$$\det\left(\Gamma - \mathbb{I}E_n\right) = 0, \tag{20a}$$

$$\frac{1}{\Psi}\frac{\partial\left|\Gamma - \mathbb{I}E_n\right|}{\partial\Psi^*} = 0. \tag{20b}$$

# Kübler's diagrams




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- Starting point:

$$S(m) = E_n - E_m^{(0)}. \qquad (21)$$

- Ascending lines:

$$L_A(m) = -\lambda J z \Psi \frac{\sqrt{m+1}}{E_n - E_m^{(0)}}. \qquad (22)$$

- Descending lines:

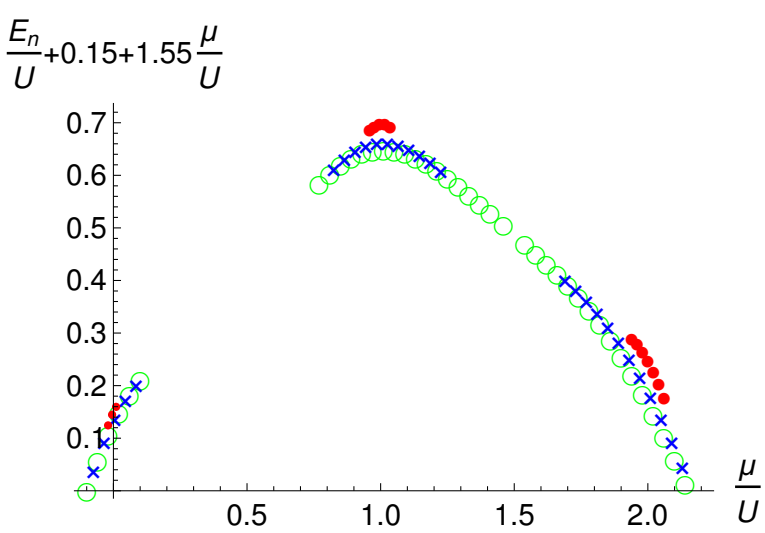
$$L_D(m) = -\lambda J z \Psi^* \frac{\sqrt{m}}{E_n - E_m^{(0)}}. \qquad (23)$$

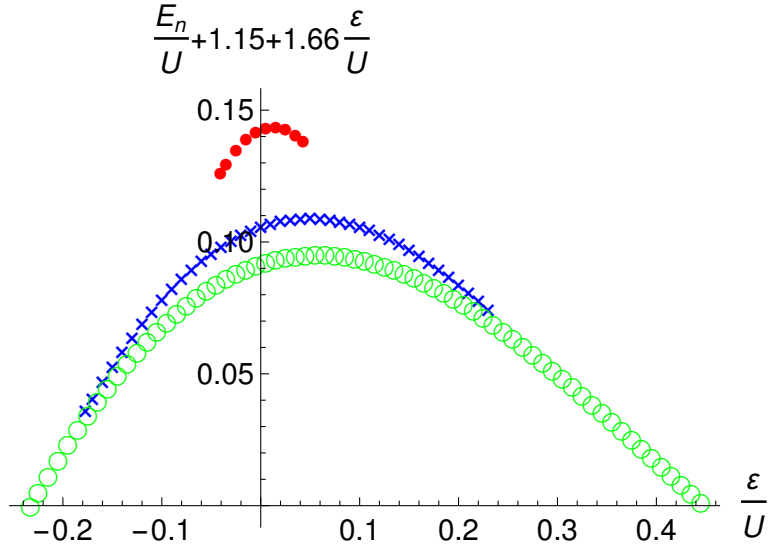
- Horizontal lines:

$$L_H(m) = \frac{\lambda J z \Psi^* \Psi}{E_n - E_m^{(0)}}. \qquad (24)$$

# Ground-state energy

- Superfluid ground-state energies $E_n/U$ for different hopping values: $Jz/U = 0.02$ (red circles), $Jz/U = 0.08$ (blue crosses), and $Jz/U = 5 - 2\sqrt{6} \approx 0.101$ (green rings).

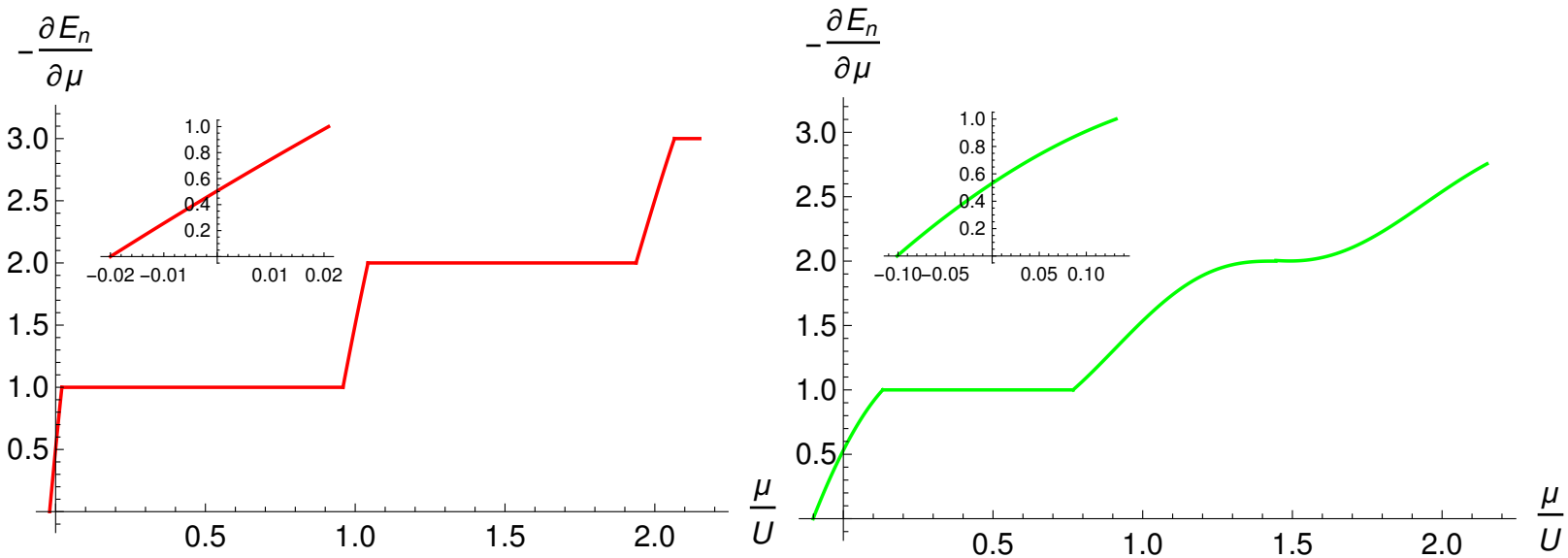



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# Particle density at T=0

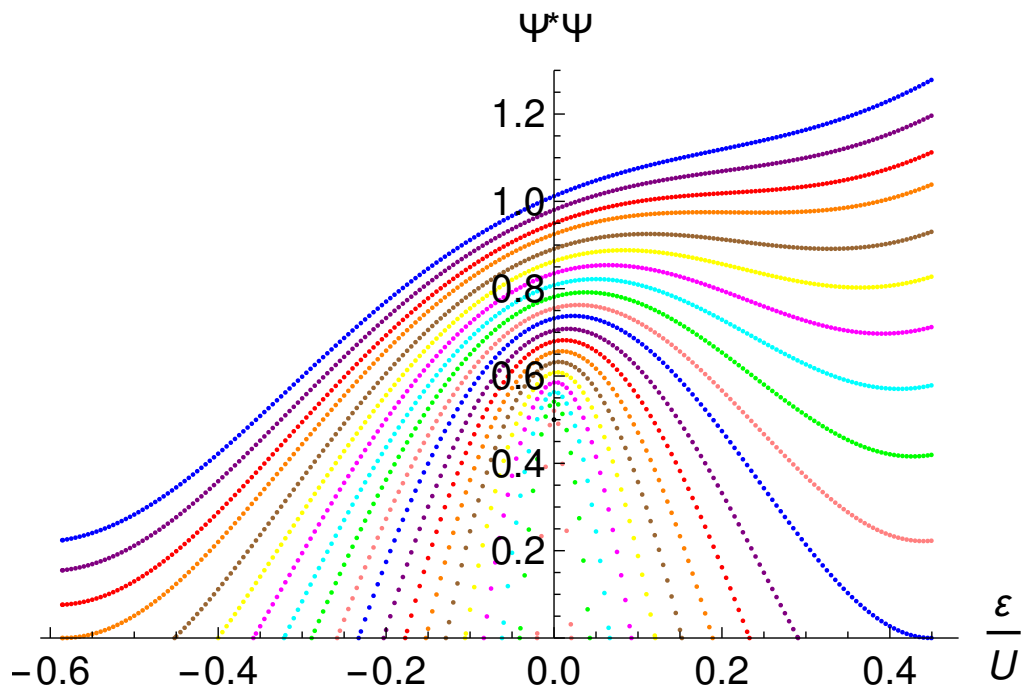
- Particle densities according to: red curve $Jz/U = 0.02$, green curve $Jz/U = 0.101$.




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# Zero-temperature condensate density

- Condensate densities $\Psi^*\Psi$ as functions of $\varepsilon/U = \mu/U - n$ for $n = 1$ up to $\lambda^4$ between the Mott lobes for different values of $Jz/U$, between $Jz/U = 0.01$ (innermost points) and $Jz/U = 0.20$ (outermost points) with a step size of 0.01.




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# Finite temperature

PHYSICAL REVIEW A **100**, 043609 (2019)

## Finite-temperature degenerate perturbation theory for bosons in optical lattices

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Bosonic atoms confined in optical lattices can exist in two different phases, Mott insulator and superfluid, depending on the strength of the system parameters, such as the on-site interaction between particles and the hopping parameter. This work is motivated by the fact that nondegenerate perturbation theory applied to the mean-field approximation of the Bose-Hubbard Hamiltonian at both zero and finite temperature fails to give consistent results in the vicinity of the Mott insulator–superfluid phase transition, e.g., the order parameter calculated via nondegenerate perturbation theory reveals an unphysical behavior between neighboring Mott lobes, which is an explicit consequence of degeneracy problems that artificially arise from such a treatment. This problem also appears in other bosonic systems that present similar Mott-lobe structures. Therefore, in order to fix this problem, we propose a finite-temperature degenerate perturbation theory approach based on a projection operator formalism which ends up solving such degeneracy problems in order to obtain physically consistent results for the order parameter near the phase transition.

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# The system at finite temperature

- Let the degenerate Hilbert subspace be $\mathcal{P}$ and its complementary subspace be $\mathcal{Q}$. Their respective projection operators are

$$\hat{\mathcal{P}} = |n\rangle\langle n| + |n+1\rangle\langle n+1|, \tag{25}$$

$$\hat{\mathcal{Q}} = \sum_{m \notin \mathcal{P}} |m\rangle\langle m|. \tag{26}$$

- Adding the operators:

$$\hat{H} = \hat{H}_0 + \left(\hat{\mathcal{P}} + \hat{\mathcal{Q}}\right) \hat{V} \left(\hat{\mathcal{P}} + \hat{\mathcal{Q}}\right). \tag{27}$$

- We define the new unperturbed Hamiltonian and the new perturbation as

$$\hat{\mathcal{H}}_0 \equiv \hat{H}_0 + \hat{\mathcal{P}}\hat{V}\hat{\mathcal{P}}, \tag{28a}$$

$$\hat{\mathcal{V}} \equiv \hat{\mathcal{P}}\hat{V}\hat{\mathcal{Q}} + \hat{\mathcal{Q}}\hat{V}\hat{\mathcal{P}} + \hat{\mathcal{Q}}\hat{V}\hat{\mathcal{Q}}. \tag{28b}$$

# Diagonalization of $\hat{\mathcal{H}}_0$

- The eigenenergies of $\hat{\mathcal{H}}_0$ are given by: $\{\ldots, E_{n-1}, \mathcal{E}_+, \mathcal{E}_-, E_{n+2}, \ldots\}$, with

$$\mathcal{E}_\pm = \frac{E_n + E_{n+1}}{2} \pm \frac{1}{2}\sqrt{\left(E_n - E_{n+1}\right)^2 + 4J^2z^2|\Psi|^2\,(n+1)}. \quad (29)$$

- While the eigenstates of $\hat{\mathcal{H}}_0$ are given by: $\{\ldots, |n-1\rangle, |\Phi_+\rangle, |\Phi_-\rangle, |n+2\rangle, \ldots\}$, with

$$|\Phi_\pm\rangle = \frac{1}{\sqrt{1 + \frac{|\mathcal{E}_\pm - E_n|^2}{J^2z^2|\Psi|^2(n+1)}}}\left[|n\rangle + \frac{E_n - \mathcal{E}_\pm}{Jz\sqrt{|\Psi|^2\,(n+1)}}|n+1\rangle\right]. \quad (30)$$

# Time-dependent perturbation theory

1. Time-dependent Schrödinger equation for the time-evolution operator:

$$\frac{d\hat{\mathcal{U}}_{\mathrm{I}}(\tau)}{d\tau} = -\hat{\mathcal{V}}_{\mathrm{I}}(\tau)\hat{\mathcal{U}}_{\mathrm{I}}(\tau). \tag{31}$$

2. Dyson series:

$$\hat{\mathcal{U}}_{\mathrm{I}}(\beta) \approx \hat{\mathcal{U}}_{\mathrm{I}}(0) - \int_0^\beta d\tau_1 \hat{\mathcal{V}}_{\mathrm{I}}(\tau_1) + \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \hat{\mathcal{V}}_{\mathrm{I}}(\tau_1)\hat{\mathcal{V}}_{\mathrm{I}}(\tau_2). \tag{32}$$

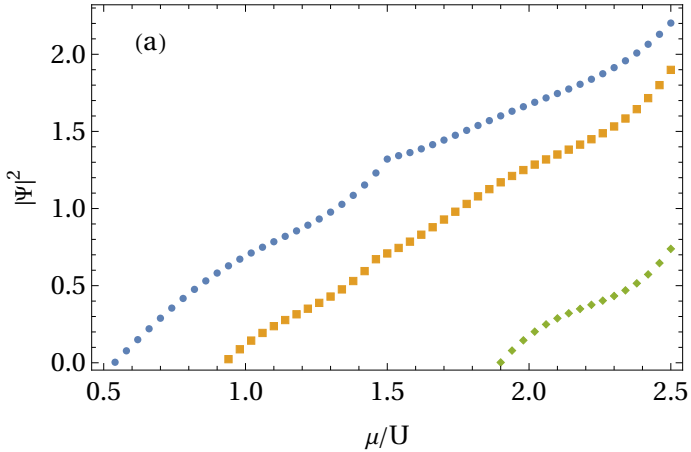
3. Goal:

$$\mathcal{F} = -\frac{1}{\beta} \log\left(\mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{\mathcal{H}}_0}\hat{\mathcal{U}}_{\mathrm{I}}(\beta)\right]\right). \tag{33}$$

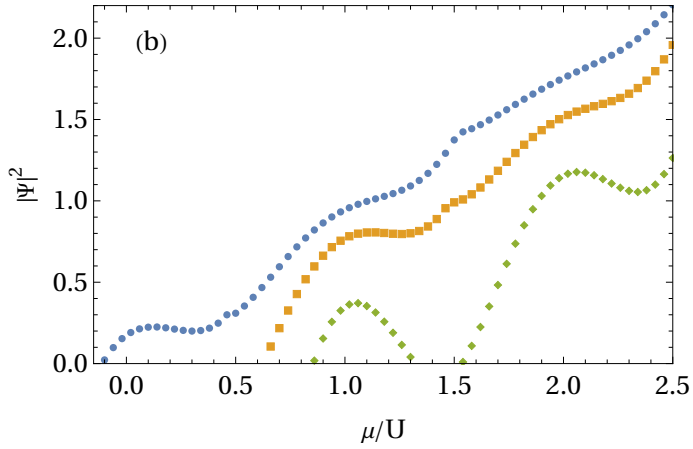
4. Condensate density:

$$\frac{\partial\mathcal{F}}{\partial|\Psi|^2} = 0. \tag{34}$$

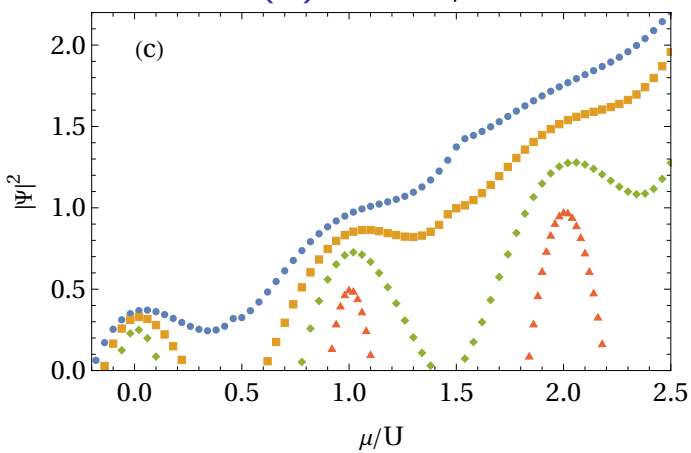
# Condensate densities



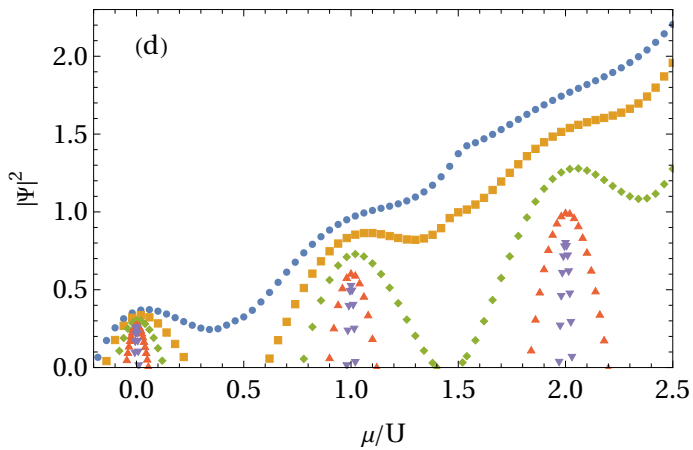

(a) $\beta = 5/U$




(b) $\beta = 10/U$



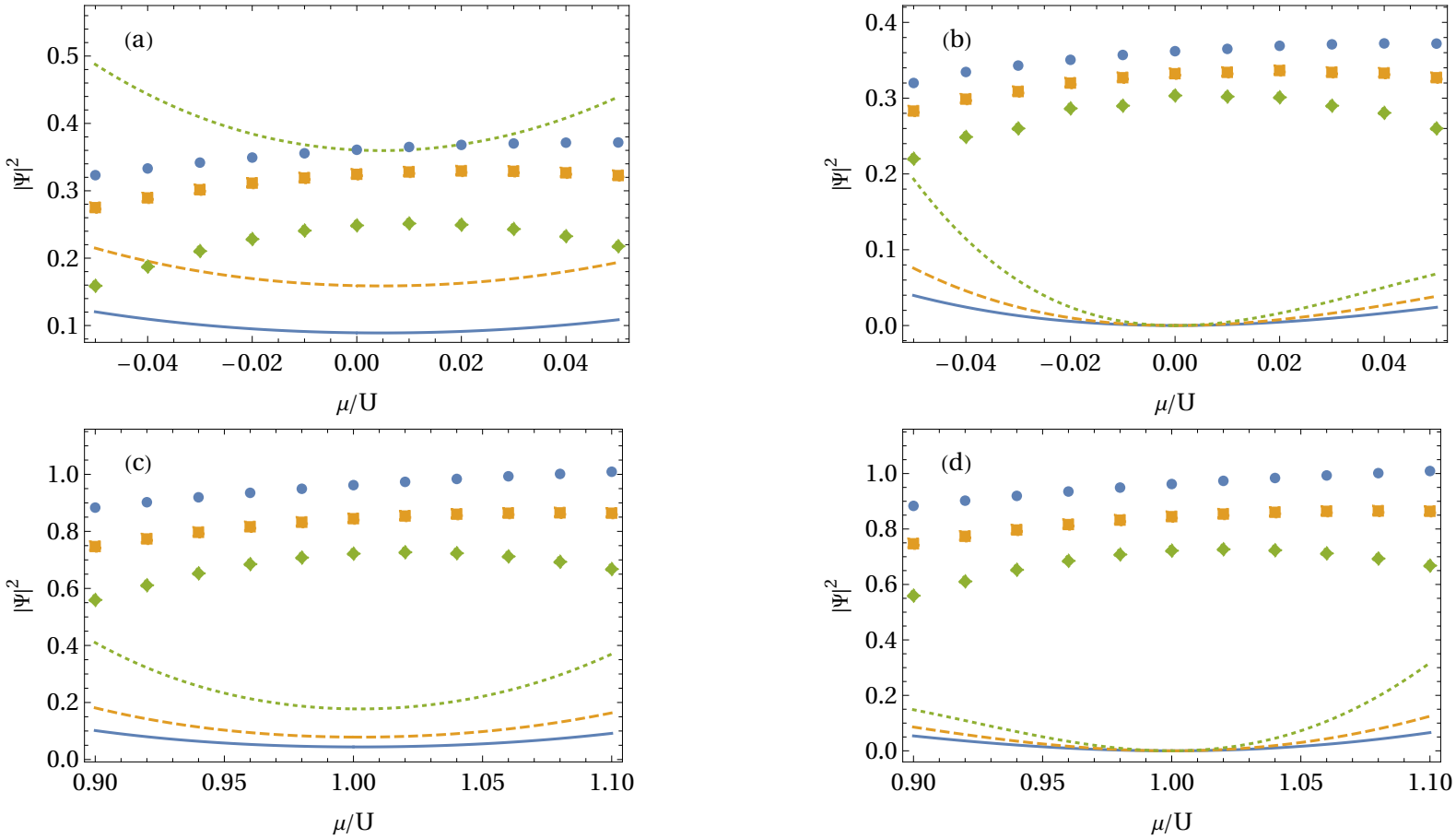

(c) $\beta = 30/U$




(d) $\beta \to \infty$

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# Comparison between NDPT and FTDPT

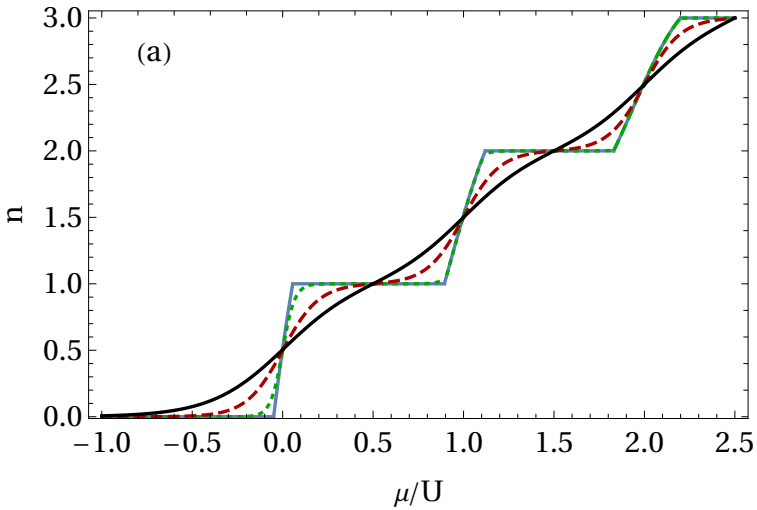



$\beta = 30/U$ $\qquad$ $T = 0$

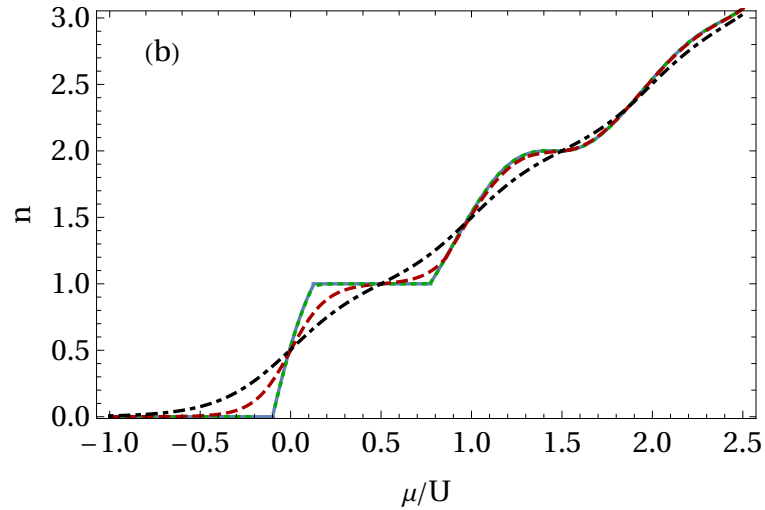
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# Particle density

- Particle densities for the temperatures $T = 0$ (continuous blue), $\beta = 30/U$ (dotted green), $\beta = 10/U$ (dashed red), and $\beta = 5/U$ (dotted-dashed black).




(a) $Jz/U = 0.05$




(b) $Jz/U = 0.1$

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# Conclusions

- We deloped a degenerate treatment based on BWPT in order to correctly calculate meaningful physical quantities, such as the energy, the condensate density, and the particle density for bosons in optical lattices at zero temperature.
- Also, for bosons at finite temperature, we developed a degenerate perturbative method based on a projection operator formalism that corrects all inconsistencies that arise from NDPT due to degeneracies that occur between two adjacent Mott lobes, which allowed to accurately evaluate the condensate densities in the vicinity of the MI-SF phase transition.
- Finally, it is important to remark that both methods not only provide relatively simple frameworks for calculating the condensate density, but are actually very generic approaches in the sense that they can also be applied to a wide range of optical-lattice systems that presents similar Mott-lobe structures.

# The interaction manifestation

- Trapped Lieb-Liniger gas of $N$ particles:

$$\hat{H} = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + V(x_i) \right) + g \sum_{i<j} \delta(x_i - x_j). \tag{35}$$

- For any pair of particles $(i, j)$:

$$\int_{-\varepsilon}^{+\varepsilon} \left[ \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_{ij}^2} + V(x_{ij}) + g\delta(x_{ij}) - E \right) \Psi(x_1, x_2, \ldots, x_N) \right] dx_{ij} = 0$$

$$\overset{\varepsilon \to 0}{\Rightarrow} -\frac{\hbar^2}{2m} \frac{\partial \Psi}{\partial x_{ij}} \Bigg|_{-\varepsilon}^{+\varepsilon} + g\Psi(x_{ij} = 0) = 0. \tag{36}$$

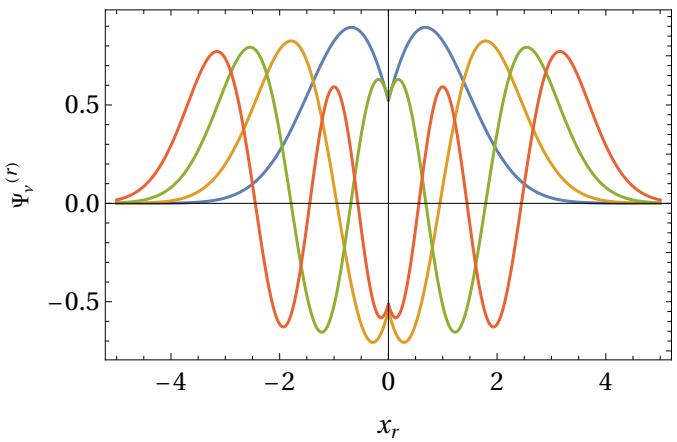
As $\varepsilon \to 0$, the contact interaction generates a condition given by

$$\left( \frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial x_j} \right) \Bigg|_{x_i - x_j \to 0^+} - \left( \frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial x_j} \right) \Bigg|_{x_i - x_j \to 0^-} = \frac{2mg}{\hbar^2} \Psi(x_i = x_j). \tag{37}$$

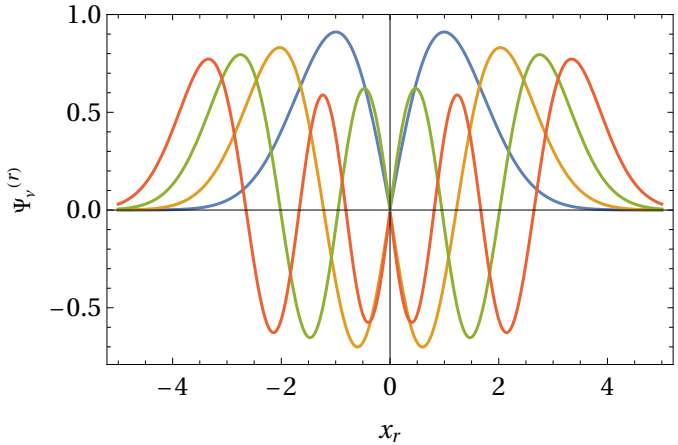
# The two-body case

- For $N = 2$ and $V(x_i) = m\omega^2 x_i^2/2$ in (35), the solutions are

$$\Psi_\nu^{(r)}(x_r) = \sqrt{\frac{1}{\mathcal{N}(\nu)}}\, \mathrm{e}^{-(x_r/a_0)^2/2}\, U\left(-\frac{\nu}{2}, \frac{1}{2}, \frac{x_r^2}{a_0^2}\right). \tag{38}$$




(a) $\tilde{g} = 1$




(b) $\tilde{g} = 100$

- Its expansion around $x = 0$ is

$$\Psi_\nu^{(r)}(x) \sim \sqrt{\frac{\pi}{\mathcal{N}(\nu)}}\left[\Gamma\left(\frac{1}{2} - \frac{\nu}{2}\right)^{-1} - 2\,\Gamma\left(-\frac{\nu}{2}\right)^{-1}\frac{|x|}{a_0} + \mathcal{O}(x^2)\right]. \tag{39}$$

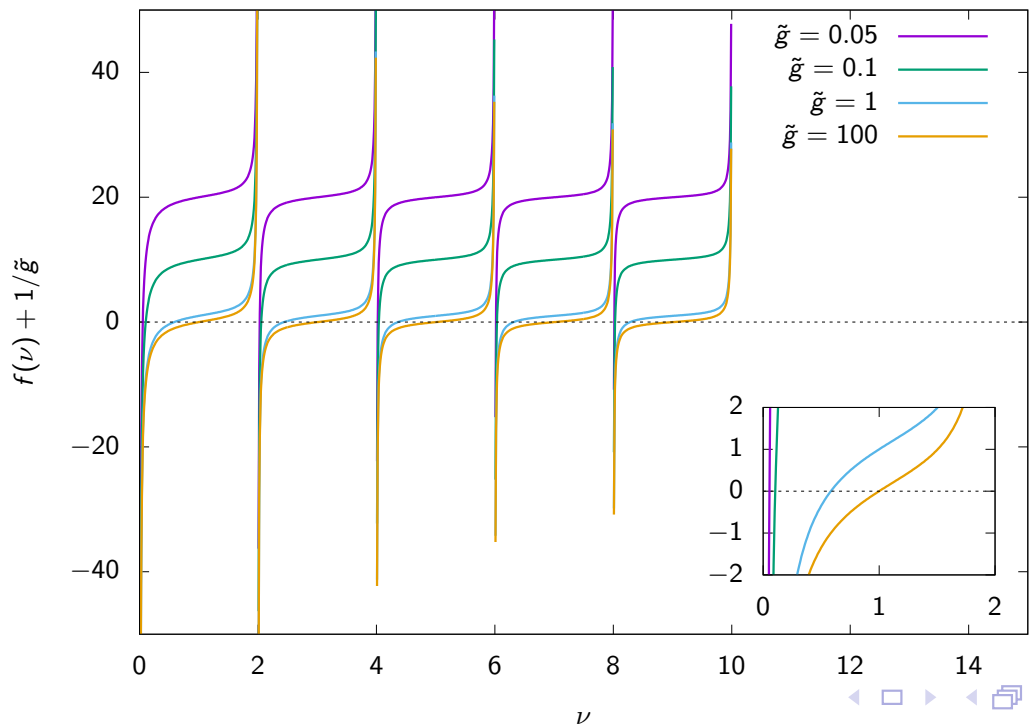
# $N = 2$ solution

- The cusp condition then reads:

$$f(\nu) \equiv \frac{\Gamma\left(-\frac{\nu}{2}\right)}{\Gamma\left(\frac{1-\nu}{2}\right)} = -\frac{1}{\tilde{g}}. \tag{40}$$

- The weakly and strongly interacting limits solutions of (40) are

$$\nu(n) = \begin{cases} 2n, & \text{for } \tilde{g} \ll 1 \\ 2n+1, & \text{for } \tilde{g} \gg 1 \end{cases}, \quad \forall\, n \in \mathbb{N}. \tag{41}$$



# Asymptotic behavior of the momentum distribution

- From the behavior of the relative motion wave function near $x_i = x_j$ (39),

$$\Psi(x_1, \ldots, x_N) \sim \Psi\left(x_1, \ldots, x_{ij}^{(cm)}, \ldots, x_N\right)\left(1 - \sqrt{2}\frac{|x_{ij}^{(r)}|}{a_{1D}}\right), \quad (42)$$

  it is possible to derive the asymptotic behavior of the momentum distribution

$$n(k) \underset{k\to\infty}{\sim} \frac{2}{\pi a_{1D}^2} k^{-4} \int dx\, \varrho^{(2)}(x, x). \quad (43)$$

- The $k^{-4}$ decay of $n(k)$ at large $k$ is a universal property of $\delta$-like interacting systems, independently of the trapping potential and the dimensionality of the system.
- Tan's contact definition:

$$\mathcal{C} \equiv \lim_{k\to\infty} k^4 n(k). \quad (44)$$

# A study on Tan's contact

PHYSICAL REVIEW A **100**, 063608 (2019)

## Scaling properties of Tan's contact: Embedding pairs and correlation effect in the Tonks-Girardeau limit

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We study Tan's contact of a one-dimensional quantum gas of $N$ repulsive identical bosons confined in a harmonic trap at finite temperature. This canonical ensemble framework corresponds to the experimental conditions, with the number of particles being fixed for each experimental sequence. We show that in the strongly interacting regime, the contact rescaled by the contact at the Tonks-Girardeau limit is a universal function of two parameters: the rescaled interaction strength and temperature. This means that all pair and correlation effects in Tan's contact are embedded in Tan's contact in the Tonks-Girardeau limit.

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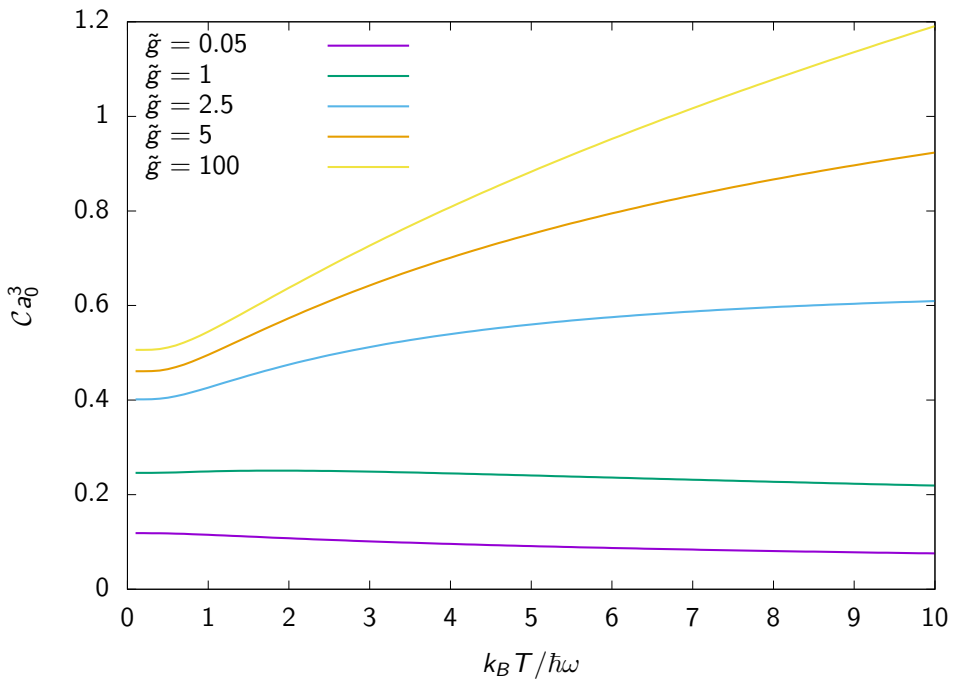
# Two-boson Tan's contact

- Tan's sweep theorem:

$$\mathcal{C} = -\frac{m^2}{\pi\hbar^4}\frac{\partial E}{\partial g^{-1}}. \tag{45}$$

- For $T > 0$:

$$\mathcal{C}(\tilde{g},\beta) = \frac{2^{5/2}\tilde{g}}{\pi a_0^3 \mathcal{Z}_r}\sum_{\nu} \mathrm{e}^{-\beta\hbar\omega\nu}\left[\psi\left(-\frac{\nu}{2}\right) - \psi\left(-\frac{\nu}{2}+\frac{1}{2}\right)\right]^{-1}. \tag{46}$$



# The Tonks-Girardeau limit

- In the strongly interacting scenario $g \to \infty$, the relationship between the many-body wave functions of the bosonic system and a fermionic one is given by [M. Girardeau, *J. Math. Phys.* **1**, 516 (1960)]

$$\Psi_\alpha^{(b)}(x_1, \ldots, x_N) = \Theta(x_1, \ldots, x_N)\Psi_\alpha^{(f)}(x_1, \ldots, x_N), \tag{47}$$

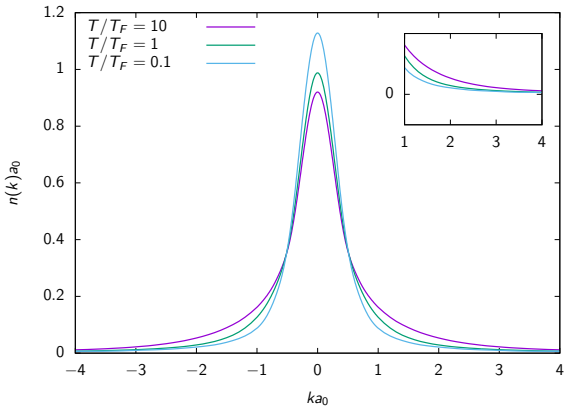
  where $\Theta(x_1, \ldots, x_N) \equiv \prod_{i>j} \mathrm{sgn}(x_i - x_j)$ is either $+1$ or $-1$, in order to compensate the anti-symmetrization of the fermionic wave function

$$\Psi_\alpha^{(f)}(x_1, \ldots, x_N) = (N!)^{-1/2} \det[\phi_{n_i}(x_j)]_{n_i \in \{n_1, \ldots, n_N\};\, x_j \in \{x_1, \ldots, x_N\}}. \tag{48}$$

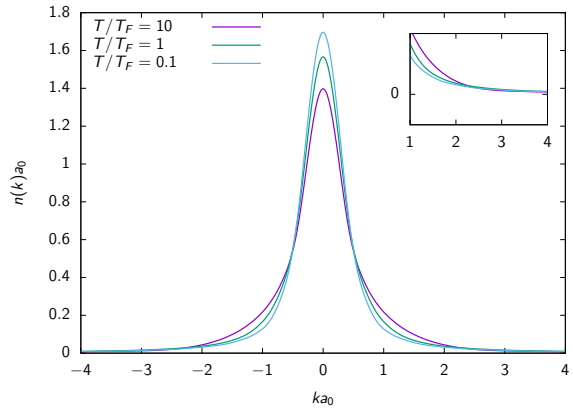
- The system constituted of strongly interacting bosons can be mapped into the ideal Fermi gas.

# Momentum distribution in the TG limit

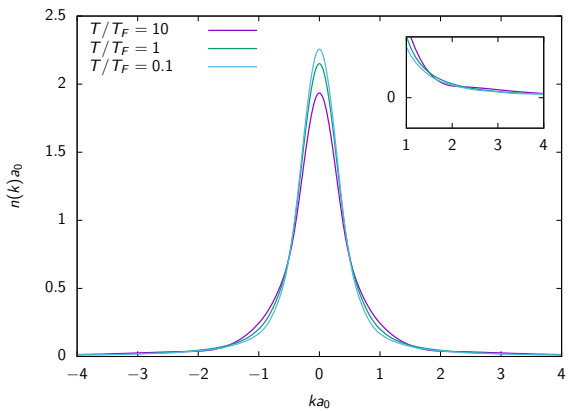
$$n(k) = \frac{1}{2\pi} \int dx \int dx' \, \mathrm{e}^{ik(x-x')} \varrho^{(1)}(x, x') \tag{49}$$



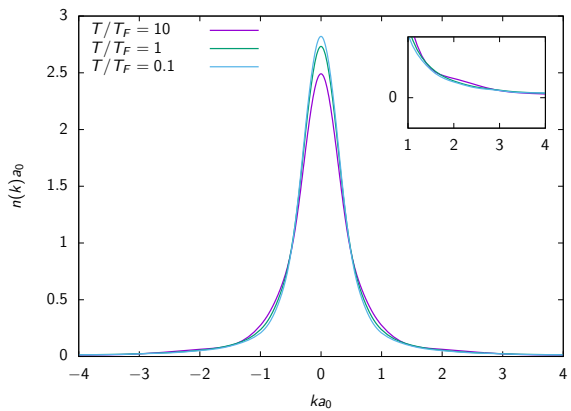

(a) $N = 2$




(b) $N = 3$



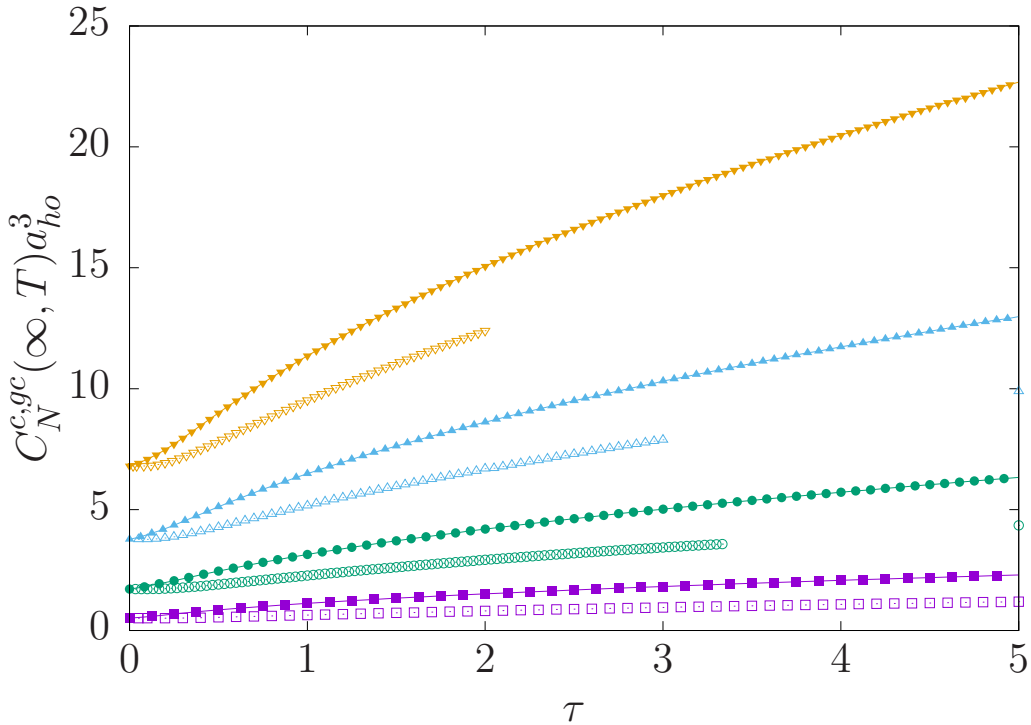

(c) $N = 4$




(d) $N = 5$

# Tonks-Girardeau Tan's contact

$$\mathcal{C} = \frac{2}{\pi}\int dx\, \mathcal{Z}^{-1} \sum_{n_1,n_2,\ldots,n_N} \mathrm{e}^{-\beta\sum_{i=1}^{N}\epsilon_{n_i}} \times \sum_{j\neq k}\left\{\left[\phi_{n_j}(x)\partial_x\phi_{n_k}(x)\right]^2 - \phi_{n_j}(x)\phi_{n_k}(x)\partial_x\phi_{n_j}(x)\partial_x\phi_{n_k}(x)\right\} \tag{50}$$




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# Zero-temperature scaling

- It was shown in [M. Rizzi *et al.*, *Phys. Rev. A* **98**, 043607 (2018)] that the contact for $N$ bosons can be expressed a function of the two-boson contact $\mathcal{C}_N = \mathcal{C}_N(\mathcal{C}_2)$. Also, it was verified that the scaling relation

$$f_N(\tilde{g}, T = 0) \equiv \frac{\mathcal{C}_N(\tilde{g}, T = 0)}{\mathcal{C}_N(\tilde{g} \to \infty, T = 0)}, \tag{51}$$

  where $\tilde{g} \equiv -a_0 a_{1\mathrm{D}}^{-1}/\sqrt{N}$ and $\mathcal{C}_N(\tilde{g}, T = 0) \propto N^{5/2} - \gamma N^{\eta}$, establishes the equality

$$f_N(\tilde{g}, T = 0) \simeq f_2(\tilde{g}, T = 0). \tag{52}$$

- In particular, in the Tonks-Girardeau limit, $\gamma \approx 1$ and $\eta = 3/4$.

# Large-temperature scaling

- For temperatures large enough, $T \gg T_F$, quantum correlations become negligible in the system, so that the contact for $N$ particles is given by the two-particle contact times the number of pairs,

$$\mathcal{C}_N(\tilde{g}, T \gg T_F) = \frac{N(N-1)}{2}\mathcal{C}_2(\tilde{g}, T \gg T_F). \tag{53}$$

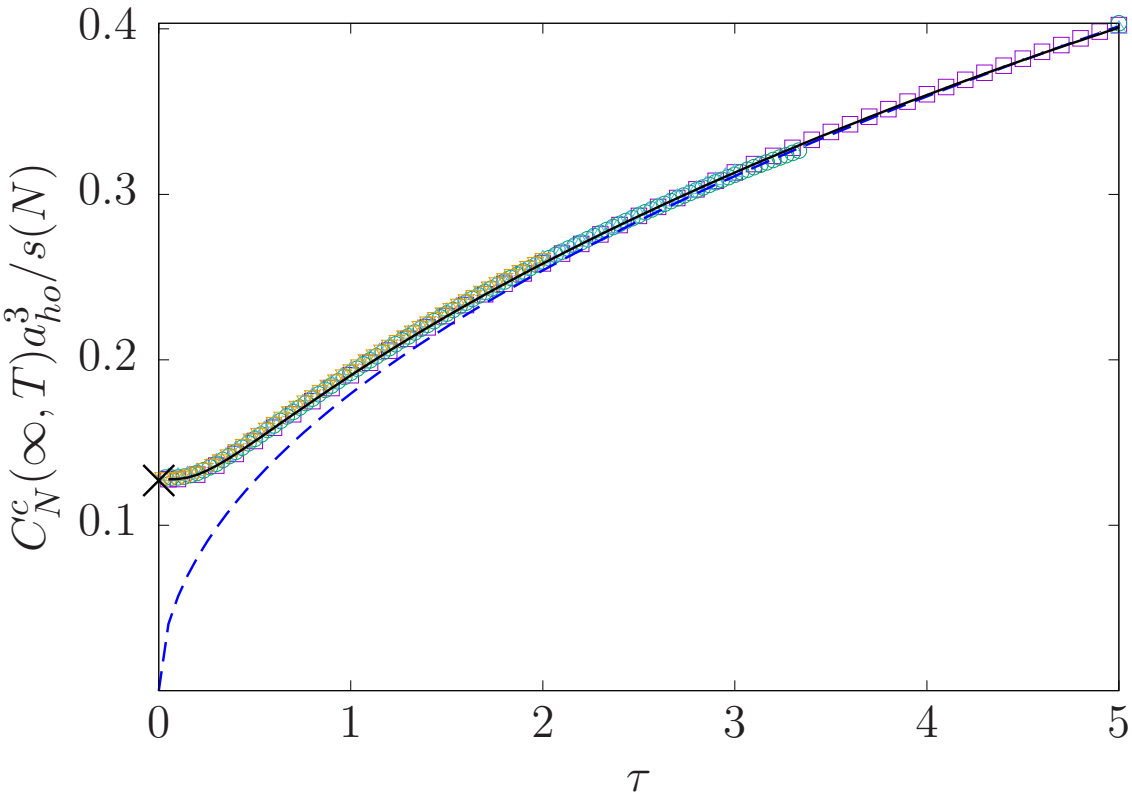
- Then, we find out that

$$\begin{aligned} &\mathcal{C}_N\left(\tilde{g} \to \infty, T \gg T_F\right) = h_N\left(\tilde{g} \to \infty, T \gg T_F\right)\left(N^{5/2} - N^{3/2}\right) \\ &\Rightarrow h_N\left(\tilde{g} \to \infty, T \gg T_F\right) = h_2(\tilde{g} \to \infty, T \gg T_F) = \frac{\sqrt{T/T_F}}{a_0^3 \pi^{3/2}}. \end{aligned} \tag{54}$$

# Generalized scaling conjecture in the TG limit

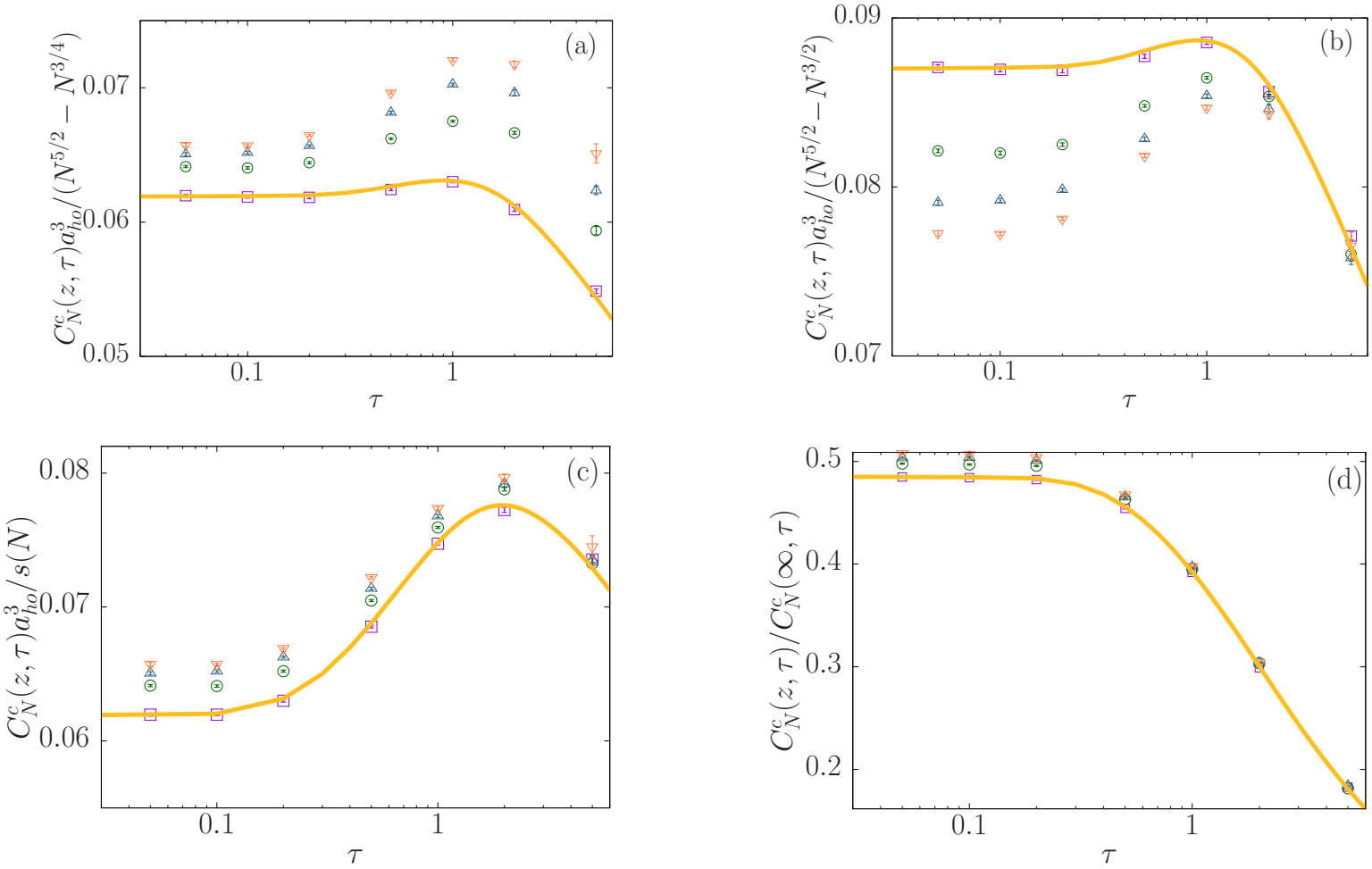
- Zero-temperature scaling: $\mathcal{C}_N(\tilde{g} \to \infty, \tau \ll 1) \propto N^{5/2} - N^{3/4}$
- Large-temperature scaling: $\mathcal{C}_N(\tilde{g} \to \infty, \tau \gg 1) \propto N^{5/2} - N^{3/2}$
- Generalized scaling conjecture:

$$\mathcal{C}_N(\tilde{g} \to \infty, \tau) \propto N^{5/2} - N^{3/4[1+\exp(-2/\tau)]} \tag{55}$$



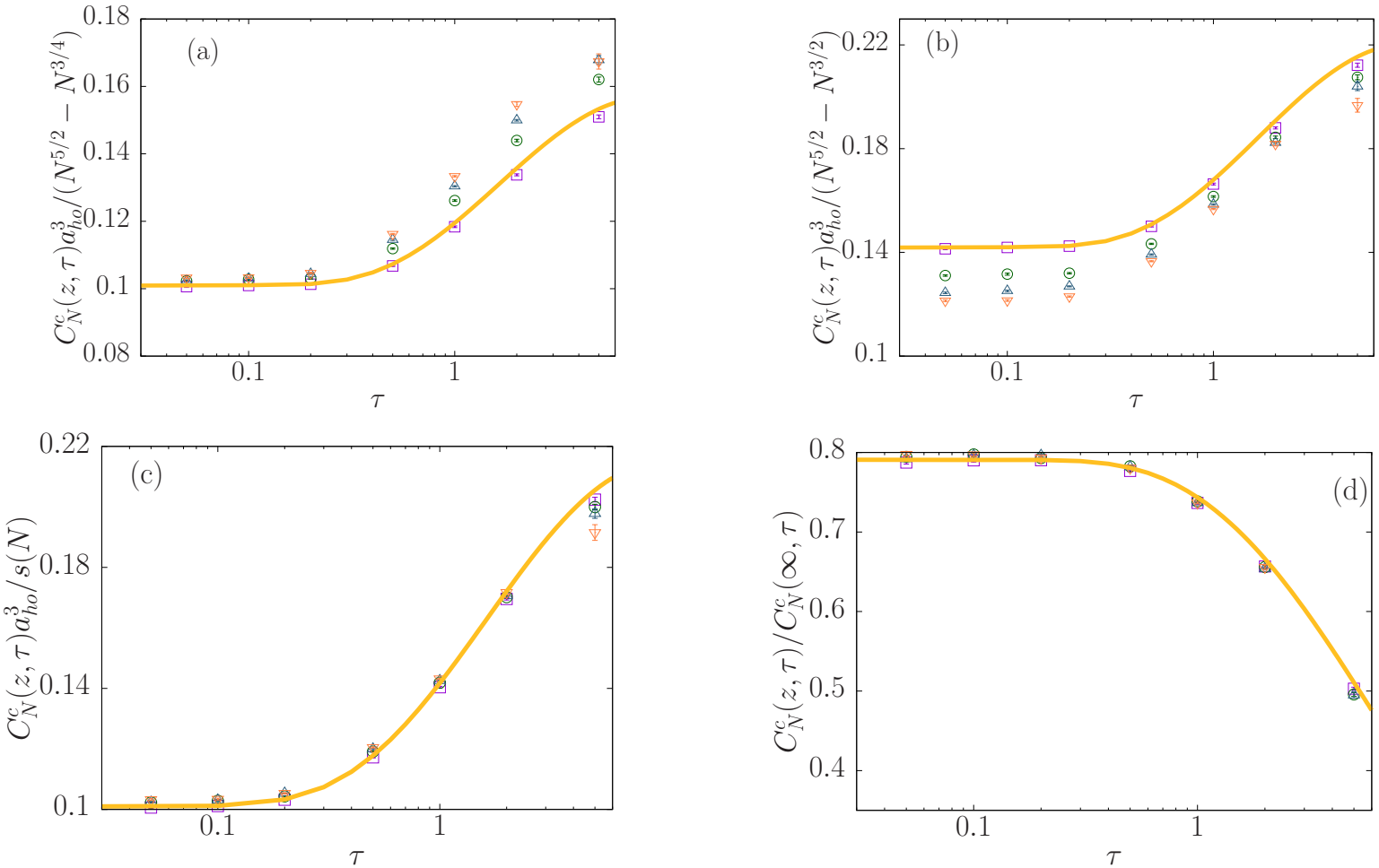

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# Intermediate-interaction scaling: $\tilde{g} = 1$




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# Intermediate-interaction scaling: $\tilde{g} = 2.5$




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# A grand-canonical consideration

- At low $T$, there is no physical distinction between the ensembles. Both scales as $N^{5/2} - N^{3/4}$.
- At large $T$, $\langle \Delta N^2 \rangle \simeq \langle N \rangle$, resulting in the average of the number of pairs $\langle N(N-1) \rangle = \langle N^2 \rangle - \langle N \rangle = \langle N \rangle^2$. Then, the contact yields

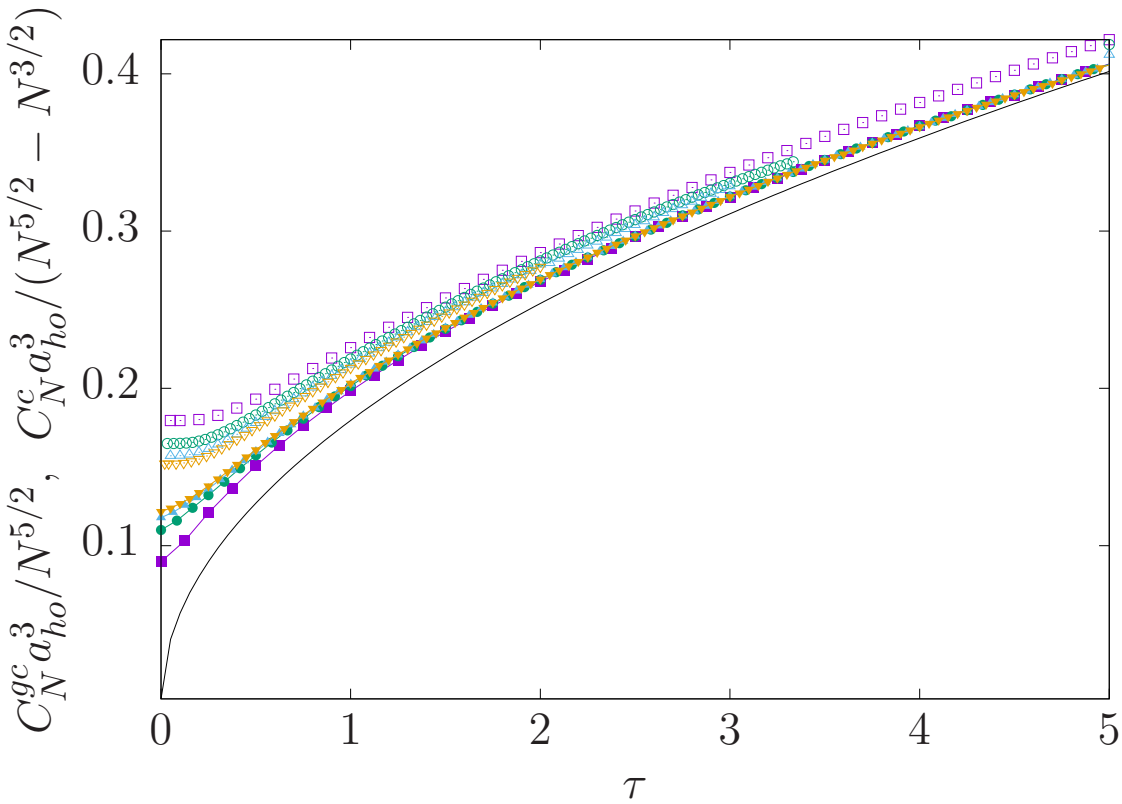
$$\mathcal{C}_N^{(gc)}(\tilde{g}, T \gg T_F) = \frac{\langle N \rangle^2}{2} \mathcal{C}_2(\tilde{g}, T \gg T_F). \tag{56}$$

- In the TG limit, the above relation yields the $\langle N \rangle^{5/2}$-dependency,

$$\mathcal{C}_N^{(gc)}(\tilde{g} \to \infty, \tau \gg 1) = \frac{\langle N \rangle^{5/2}}{\pi^{3/2} a_0^3} \sqrt{\tau}. \tag{57}$$

# A comparison between ensembles

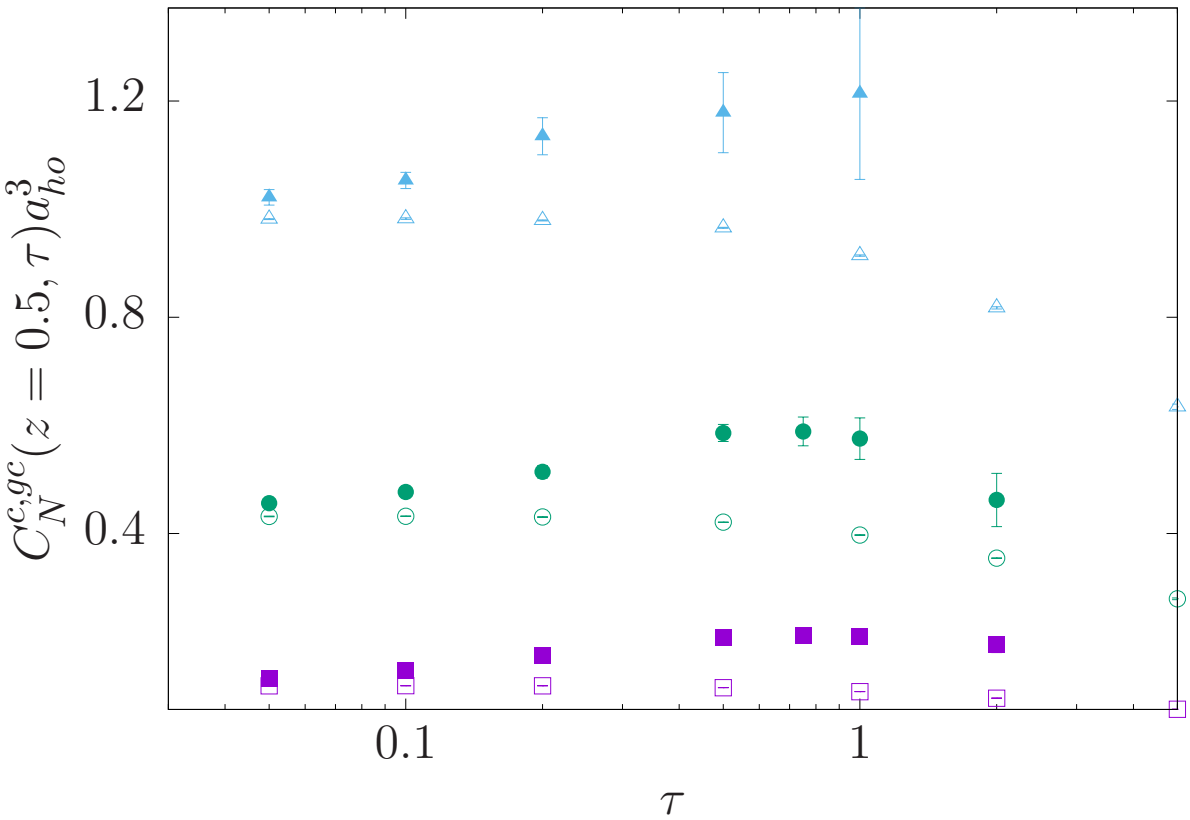
- Canonical (empty symbols) contact in the TG limit from (50) and grand-canonical (filled symbols) contact from P. Vignolo and A. Minguzzi, *Phys. Rev. Lett.* **110**, 020403 (2013).




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# Grand-canonical QMC results

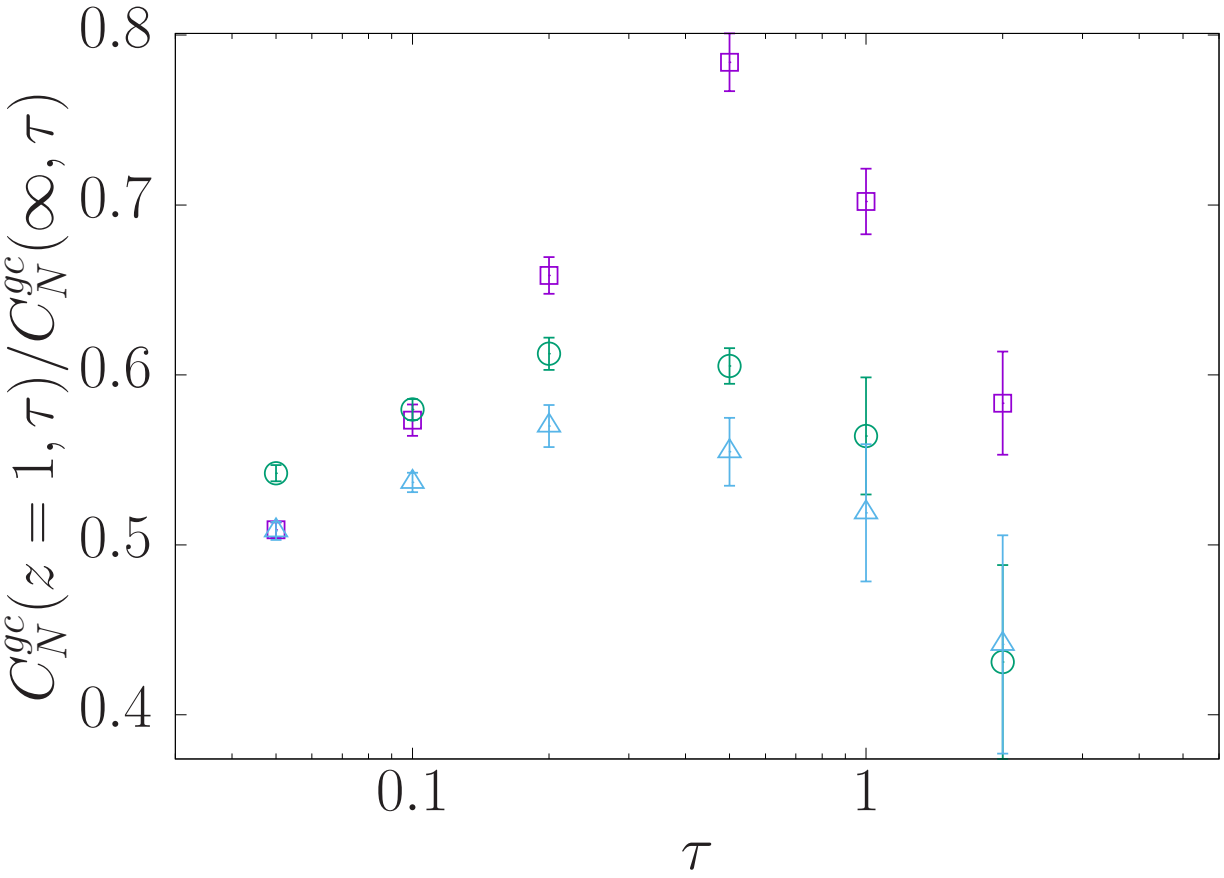
- Tan's contact evaluated from canonical QMC simulations (empty symbols) and from grand-canonical QMC simulations (filled symbols).




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# Grand-canonical QMC scaling

- QMC grand-canonical contact rescaled by the TG grand-canonical contact from P. Vignolo *et al.*, *Phys. Rev. Lett.* **110**, 020403 (2013).




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# Conclusions

- We developed an analytical formula for calculating the canonical Tan's contact in the Tonks-Girardeau limit for an interacting Bose gas under harmonic confinement.
- Then, we studied the scaling properties of the contact:
  1. Firstly, we worked out a large temperature scaling at the TG limit.
  2. Then, also at the TG limit, we proposed a generalized scaling conjecture for the whole range of temperatures, that works very well for any $T$.
  3. Afterwards, relying on QMC simulations, we showed that all previously stated scalings in the TG limit also apply for the intermediate interaction regime.
  4. Summary: The contact rescaled by the generalized scaling function and the ratio between the finite-interaction contact and its correspondent in the Tonks-Girardeau limit are both universal functions of $\tilde{g}$ and $\tau$.
  5. Comparison between ensembles: at large $T$, both the canonical and the grand-canonical contacts are proportional to the two-boson contact. The TG scaling was not confirmed for the grand-canonical ensemble for $\tilde{g} \sim 1$ at intermediate and small $T$.

# People involved



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# Thanks!