Correlation aspects of interacting quantum systems in reduced dimensionality

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Summary

Free Lieb-Liniger

arXiv:2104.10491

- One-body correlation function
- Form factors

Trapped Lieb-Liniger

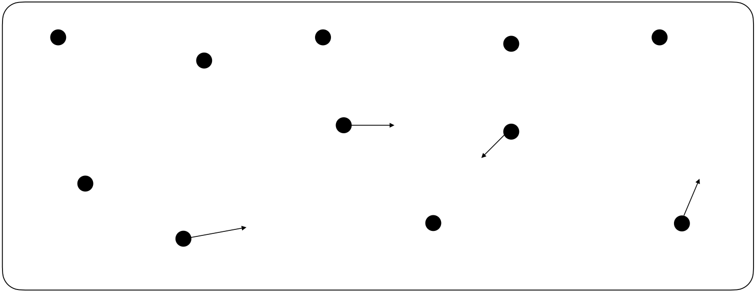
arXiv:1908.08714

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

Bosons in optical lattices

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

Wonders of one-dimensional world



Some physical peculiarities

- Landau-Fermi liquid theory, describing interacting electrons, breaks down in one dimension[1]: 1d analogue is the Tomonaga-Luttinger theory [2];
- There is no $U(1)$-symmetry breaking in 1d (HMW theorem);
- No BEC occurs for infinite systems at $T > 0$ in $d \leq 2$ (spatial confinement restores BEC occurrence);
- ...

[1] LANDAU, L. D. The theory of a Fermi liquid. Journal of Experimental and Theoretical Physics, v. 30, n. 6, p. 920, 1956

[2] LUTTINGER, J. M. An exactly soluble model of a many-fermion system. Journal of Mathematical Physics, v. 4, n. 9, p. 1154-1162, 1963

Section 1

Free Lieb-Liniger

arXiv:2104.10491

Interacting bosonic particles in 1d

- Point-like interaction:

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

- Solved by Lieb and Liniger in 1960 via Bethe ansatz considerations
- Upon imposing periodic boundary conditions, the rapidities are provided by the Bethe equations

$$\lambda_j + \frac{2}{L}\sum_{\ell=1}^{N}\arctan\left(\frac{\lambda_j - \lambda_\ell}{c}\right) = \frac{2\pi}{L}I_j, \quad j = 1, \dots, N, \tag{2}$$

  where we identitfy I_j's as quantum numbers, that can be either integers (odd N) or half-odd integers (even N). The ground-state is given by the Fermi sea,

$$I_j = j - (N+1)/2, \quad j = 1, \dots, N. \tag{3}$$

- The energy and momentum of a given eigenstate are $E_{\boldsymbol{\lambda}} = \sum_{j=1}^{N}\lambda_j^2, \qquad P_{\boldsymbol{\lambda}} = \sum_{j=1}^{N}\lambda_j.$

Strongly repulsive regime

When $c \to \infty$, we reach the Tonks-Girardeau gas:

- Strong repulsion between particles plays the role of the Pauli exclusion principle;
- The bosonic system can be mapped into the fermionic one, *fermionization*;
- Energy spectra are equal, whereas wave functions are not, but there is a correspondence;
- At $c \to \infty$ the Bethe equations (2) decouple to simple quantization conditions
$$\lambda_j = \frac{2\pi}{L} I_j, \qquad j = 1, \ldots, N. \tag{4}$$

One-body function

- One-body correlation function over the ground state

$$g(x,t) = \langle \boldsymbol{\lambda} | \Psi^\dagger(x,t)\Psi(0,0) | \boldsymbol{\lambda} \rangle. \tag{5}$$

- Time evolution:

$$g(x,t) = \sum_{\boldsymbol{\mu} \in \mathcal{H}_{N-1}} e^{-i(E_{\boldsymbol{\lambda}} - E_{\boldsymbol{\mu}})t + i(P_{\boldsymbol{\mu}} - P_{\boldsymbol{\lambda}})x} |\langle \boldsymbol{\mu} | \Psi(0) | \boldsymbol{\lambda} \rangle|^2, \tag{6}$$

  where the space- and time-independent term, $|\langle \boldsymbol{\mu} | \Psi(0) | \boldsymbol{\lambda} \rangle|^2$, is the so-called form factor.

- TG: A milestone is the exact result from Lenard [3]

$$g(x) = \det_N(I + V_1 + V_2) - \det_N(I + V_1), \tag{7}$$

  where I is the identity matrix and

$$V_1^{ij} = -\frac{4}{L}\frac{\sin(x(k_i - k_j)/2)}{(k_i - k_j)}, \qquad V_2^{ij} = \frac{1}{L}e^{-ix(k_i+k_j)/2}, \tag{8}$$
$$i, j = 1, \dots, N.$$

[3] A. Lenard, *Momentum Distribution in the Ground State of the One-Dimensional system of Impenetrable Bosons*, *J. Math. Phys.* **5** (1964) 930–943.

Form factors

- The field operator form factor for the Lieb-Liniger, can be formulated as[4]

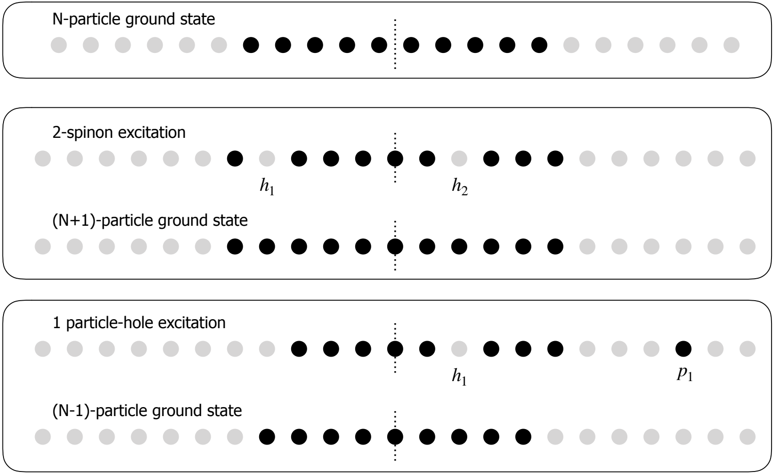
$$|\langle \boldsymbol{\mu}|\Psi(0)|\boldsymbol{\lambda}\rangle|^2 = c^{2N-1}\frac{\prod_{j>k=1}^{N}\left(\lambda_{jk}^2+c^2\right)^2}{\prod_{j=1}^{N}\prod_{k=1}^{N-1}\left(\lambda_j-\mu_k\right)^2}\frac{\det_{N-1}^2 U(\boldsymbol{\mu},\boldsymbol{\lambda})}{\|\boldsymbol{\mu}\|^2\|\boldsymbol{\lambda}\|^2}. \quad (9)$$

- The limit $c\to\infty$ of the form factor (9) is given by

$$|\langle \boldsymbol{\mu}|\Psi(0)|\boldsymbol{\lambda}\rangle|^2 = \frac{1}{2}\left(\frac{2}{L}\right)^{2N-1}\frac{\prod_{j>k=1}^{N}(\lambda_j-\lambda_k)^2\prod_{j>k=1}^{N-1}(\mu_j-\mu_k)^2}{\prod_{j=1}^{N}\prod_{k=1}^{N-1}\left(\lambda_j-\mu_k\right)^2}. \quad (10)$$

[4] V. E. Korepin, N. M. Bogoliubov and A. G. Izergin, Quantum Inverse Scattering Method and Correlation Functions. Cambridge Univ. Press, Cambridge, 1993.

Elementary excitations



Momentum aftermath

- Momentum change of the system:

$$\Delta k_{2sp} \equiv k_{2sp}^{(N-1)} - k_{GS}^{(N+1)} = \frac{2\pi}{L}\left(\sum_{\substack{j=1\\ j\neq h_1,h_2}}^{N+1} I_j^{(N+1)} - \sum_{j=1}^{N+1} I_j^{(N+1)}\right) \tag{11}$$

$$= -\frac{2\pi}{L}\left(I_{h_1}^{(N+1)} + I_{h_2}^{(N+1)}\right).$$

- We define the momentum of the two-spinon excitation as the difference between the excited and the ground states with the same number of particles,

$$k_{2sp} \equiv k_{2sp}^{(N-1)} - k_{GS}^{(N-1)} = \frac{2\pi}{L}\left(\sum_{\substack{j=1\\ j\neq h_1,h_2}}^{N+1} I_j^{(N+1)} - \sum_{j=1}^{N-1} I_j^{(N-1)}\right). \tag{12}$$

  Thence, we have that

$$k_{2sp} = -\frac{2\pi}{L}\left(I_{h_1}^{(N+1)} + I_{h_2}^{(N+1)}\right). \tag{13}$$

- The momentum of the excitation is equal to the momentum change.

Energy aftermath

- Energy change in the system:

$$\Delta\omega_{2sp} \equiv \omega_{2sp}^{(N-1)} - \omega_{GS}^{(N+1)} = \left(\frac{2\pi}{L}\right)^2 \left(\sum_{\substack{j=1 \\ j\neq h_1,h_2}}^{N+1} \left(I_j^{(N+1)}\right)^2 - \sum_{j=1}^{N+1} \left(I_j^{(N+1)}\right)^2 \right)$$
$$= -\left(\frac{2\pi}{L}\right)^2 \left[\left(I_{h_1}^{(N+1)}\right)^2 + \left(I_{h_2}^{(N+1)}\right)^2\right]. \tag{14}$$

- Excitation energy:

$$\omega_{2sp} \equiv \omega_{2sp}^{(N-1)} - \omega_{GS}^{(N-1)} = \left(\frac{2\pi}{L}\right)^2 \left(\sum_{\substack{j=1 \\ j\neq h_1,h_2}}^{N+1} \left(I_j^{(N+1)}\right)^2 - \sum_{j=1}^{N-1} \left(I_j^{(N-1)}\right)^2 \right)$$
$$= -\left(\frac{2\pi}{L}\right)^2 \left[\left(I_{h_1}^{(N+1)}\right)^2 + \left(I_{h_2}^{(N+1)}\right)^2 - \frac{N^2}{2}\right]. \tag{15}$$

- The energy of the excitation is greater than the energy change

$$\omega_{2sp} = \Delta\omega_{2sp} + 2\epsilon_F. \tag{16}$$

Form factors of two spinons

- A generic excited state consists of two spinons parametrized by the positions of the two holes, (h_1, h_2), and m particle-hole excitations, each described by a pair (p_j, h_j) with $j = 3, \ldots, m+2$. In this fashion the form factor (10) becomes

$$|\langle \boldsymbol{\mu}|\Psi(0)|\boldsymbol{\lambda}\rangle|^2 = \Omega(L,N) \times \prod_{a=1}^{m+2} \frac{\prod_{j=1}^{N}(\lambda_j - h_a)^2}{\prod_{j=1}^{N+1}(\bar{\mu}_j - h_a)^2} \prod_{a=3}^{m+2} \frac{\prod_{j=1}^{N+1}(\bar{\mu}_j - p_a)^2}{\prod_{j=1}^{N}(\lambda_j - p_a)^2}$$
$$\times \frac{\prod_{a>b=3}^{m+2}(h_a - h_b)^2 \prod_{a>b=1}^{m+2}(p_a - p_b)^2}{\prod_{a=1}^{m+2}\prod_{b=3}^{m+2}(h_a - p_b)^2}. \tag{17}$$

where

$$\Omega(N,L) = \frac{1}{2}\left(\frac{2}{L}\right)^{2N-1} \frac{\prod_{j>k=1}^{N}(\lambda_j - \lambda_k)^2 \prod_{j>k=1}^{N+1}(\bar{\mu}_j - \bar{\mu}_k)^2}{\prod_{j=1}^{N}\prod_{k=1}^{N+1}(\lambda_j - \bar{\mu}_k)^2}$$
$$= \frac{L}{4} G^4(3/2)\left[\frac{G(N+1)G(N+2)}{G^2(N+3/2)}\right]^2, \tag{18}$$

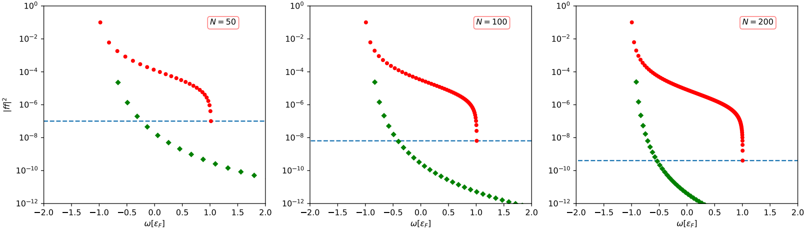
is a factor which is independent of the excited state.

Further particle-hole excitations

- Consider a further particle-hole excitation over the excited state $|\boldsymbol{\mu}\rangle$ (2sp+$m$ph), i.e., $|\boldsymbol{\mu} + (p_{m+3}, h_{m+3})\rangle$. It is possible to show that ratio between the respective form factors is less than 1,

$$|\langle \boldsymbol{\mu} + (p_{m+3}, h_{m+3})|\Psi(0)|\boldsymbol{\lambda}\rangle|^2 < |\langle \boldsymbol{\mu}|\Psi(0)|\boldsymbol{\lambda}\rangle|^2. \qquad (19)$$

- Form factors for two classes of excitations. The form factors with two-spinon excitations (red) are larger than the form factors for 2ph on top of 2sp (green).



arXiv:2104.10491

Two-spinon one-body function

- The two-spinon one-body function is given by,

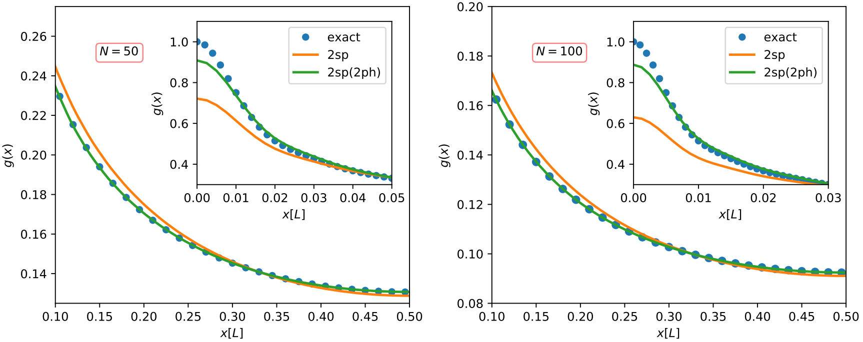
$$g_{2\mathrm{sp}}(x,t) = \sum_{|\alpha\rangle \in \mathcal{H}_{2sp}} e^{i\omega_{2\mathrm{sp}}(\alpha)t - ik_{2\mathrm{sp}}(\alpha)x} |\langle \alpha | \Psi(0) | \mathrm{GS} \rangle|^2. \tag{20}$$

where the 2sp form factor is equivalent to (17) for $m = 0$, i.e.,

$$|\langle \boldsymbol{\mu} | \Psi(0) | \boldsymbol{\lambda} \rangle|^2 = \Omega(L,N) \times \frac{\prod_{j=1}^{N}(\lambda_j - h_1)^2}{\prod_{j=1}^{N+1}(\bar{\mu}_j - h_1)^2} \frac{\prod_{j=1}^{N}(\lambda_j - h_2)^2}{\prod_{j=1}^{N+1}(\bar{\mu}_j - h_2)^2} (h_1 - h_2)^2, \tag{21}$$

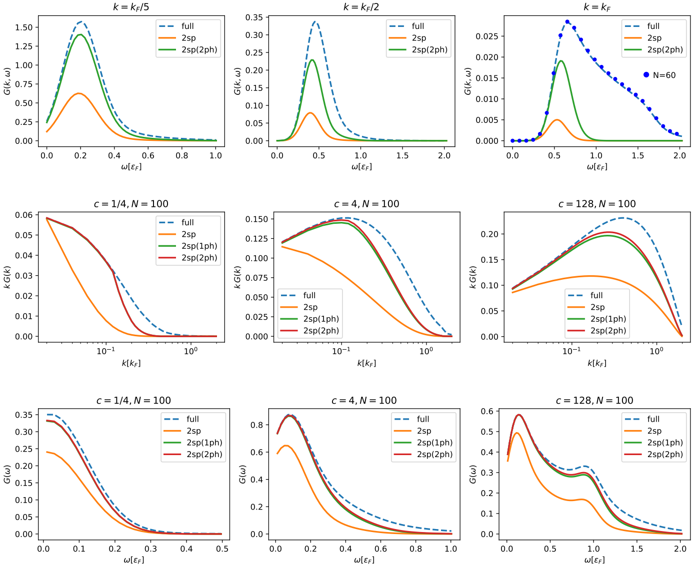
and the sum extends over possible choices of the two holes (h_1, h_2) in the $(N+1)$-particle ground state. The rapidities λ_j and $\bar{\mu}_j$ are respectively ground-state rapidities of systems with N and $N+1$ particles.

2sp one-body function in TG regime



M. Panfil, F.T. Sant'Ana, arXiv:2104.10491

Finite interaction: ABACUS[5]



[5] J.-S. Caux, arXiv:0908.1660

Finite temperature generalization

The generalization for finite-temperature correlation function of bosons in the Tonks-Girardeau gas can be evaluated through [6]

$$\langle \Psi^\dagger(x_2, t_2)\Psi(x_1, t_1)\rangle = e^{i\mu t_{21}} \left(\frac{1}{2\pi} G'(t_{12}, x_{12}) + \frac{\partial}{\partial \alpha} \right) \det(1 + \hat{V}) \Big|_{\alpha=0} \tag{22}$$

where $t_{12} \equiv t_1 - t_2$ and $x_{12} \equiv x_1 - x_2$. Also

$$V = \exp\left\{ -\frac{i}{2} t_{12}(q_1^2 + q_2^2) + \frac{i}{2} x_{12}(q_1 + q_2) \right\} \tag{23}$$

$$\sqrt{n(q1)n(q2)} \left[\frac{E(q_1) - E(q_2)}{\pi^2(q_1 - q_2)} - \frac{\alpha}{2\pi^3} E(q_1)E(q_2) \right] \tag{24}$$

with

$$G'(t_{12}, x_{12}) = \int_{-\infty}^{+\infty} e^{it_{12}k^2 - ix_{12}k} dk \tag{25}$$

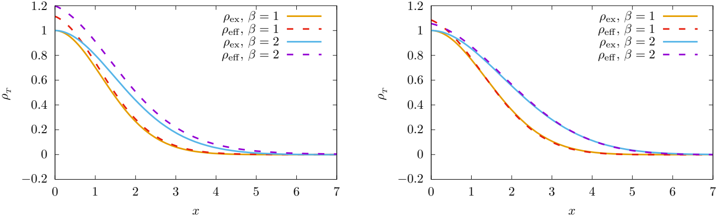
and

$$E(q, t_{12}, x_{12}) = \fint_{-\infty}^{+\infty} dk \, \frac{e^{it_{12}k^2 - ix_{12}k}}{k - q}. \tag{26}$$

[6] arxiv:0912.3633

Impurity in noninteracting gas

$$H = \frac{P_{\rm imp}^2}{2m} + \sum_{j=1}^{N} \frac{P_j^2}{2m} + g \sum_{j=1}^{N} \delta(x_j - x_{\rm imp}). \qquad (27)$$



O. Gamayun, M. Panfil, F.T. Sant'Ana, arXiv:2202.07657

Section 2

Trapped Lieb-Liniger

arXiv:1908.08714

The interaction manifestation

- Trapped Lieb-Liniger gas of N particles:

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + V(x_i) \right) + g \sum_{i<j} \delta(x_i - x_j). \tag{28}$$

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

$$\int_{-\varepsilon}^{+\varepsilon} \left[\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_{ij}^2} + V(x_{ij}) + g\delta(x_{ij}) - E \right) \Psi\left(x_1, x_2, \ldots, x_N\right) \right] dx_{ij} = 0$$
$$\overset{\varepsilon \to 0}{\Rightarrow} -\frac{\hbar^2}{2m} \frac{\partial \Psi}{\partial x_{ij}} \bigg|_{-\varepsilon}^{+\varepsilon} + g\Psi\left(x_{ij} = 0\right) = 0. \tag{29}$$

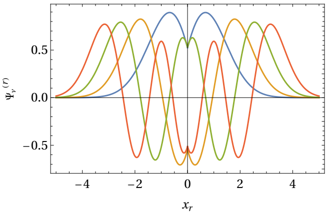
As $\varepsilon \to 0$, the contact interaction generates a condition given by

$$\left(\frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial x_j} \right) \bigg|_{x_i - x_j \to 0^+} - \left(\frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial x_j} \right) \bigg|_{x_i - x_j \to 0^-} = \frac{2mg}{\hbar^2} \Psi(x_i = x_j). \tag{30}$$

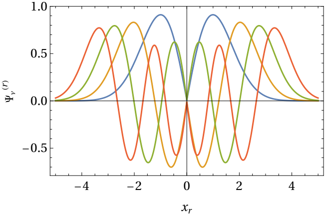
The two-body case

- For $N = 2$ and $V(x_i) = m\omega^2 x_i^2/2$ in (28), the solutions are

$$\Psi_\nu^{(r)}(x_r) = \sqrt{\frac{1}{\mathcal{N}(\nu)}}\, \mathrm{e}^{-(x_r/a_0)^2/2}\, U\left(-\frac{\nu}{2}, \frac{1}{2}, \frac{x_r^2}{a_0^2}\right). \qquad (31)$$



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



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

- Its expansion around $x = 0$ is

$$\Psi_\nu^{(r)}(x) \sim \sqrt{\frac{\pi}{\mathcal{N}(\nu)}} \left[\Gamma\left(\frac{1}{2} - \frac{\nu}{2}\right)^{-1} - 2\,\Gamma\left(-\frac{\nu}{2}\right)^{-1} \frac{|x|}{a_0} + \mathcal{O}(x^2) \right]. \qquad (32)$$

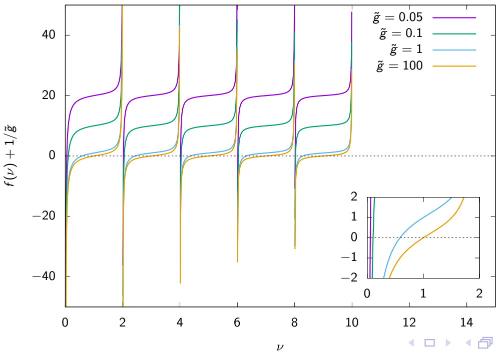
$N = 2$ solution

- The cusp condition then reads:

$$f(\nu) \equiv \frac{\Gamma\left(-\frac{\nu}{2}\right)}{\Gamma\left(\frac{1-\nu}{2}\right)} = -\frac{1}{\tilde{g}}. \tag{33}$$

- The weakly and strongly interacting limits solutions of (33) are

$$\nu(n) = \begin{cases} 2n, & \text{for } \tilde{g} \ll 1 \\ 2n+1, & \text{for } \tilde{g} \gg 1 \end{cases}, \quad \forall\, n \in \mathbb{N}. \tag{34}$$



Asymptotic behavior of the momentum distribution

- From the behavior of the relative motion wave function near $x_i = x_j$ (32),

$$\Psi(x_1, \ldots, x_N) \sim \Psi\left(x_1, \ldots, x_{ij}^{(cm)}, \ldots, x_N\right)\left(1 - \sqrt{2}\frac{|x_{ij}^{(r)}|}{a_{1\mathrm{D}}}\right), \quad (35)$$

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

$$n(k) \underset{k\to\infty}{\sim} \frac{2}{\pi a_{1\mathrm{D}}^2} k^{-4} \int dx \, \varrho^{(2)}(x, x). \quad (36)$$

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

$$\mathcal{C} \equiv \lim_{k\to\infty} k^4 n(k). \quad (37)$$

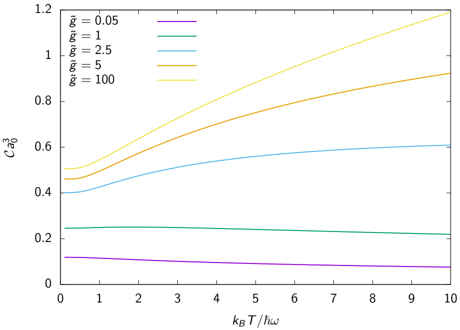
Two-boson contact

- In terms of energy it can be written as

$$\mathcal{C} = -\frac{m^2}{\pi\hbar^4}\frac{\partial E}{\partial g^{-1}}. \tag{38}$$

- For $T > 0$:

$$\mathcal{C}(\tilde{g},\beta) = \frac{2^{5/2}\tilde{g}}{\pi a_0^3 \mathcal{Z}_r}\sum_{\nu} \mathrm{e}^{-\beta\hbar\omega\nu}\left[\psi\left(-\frac{\nu}{2}\right) - \psi\left(-\frac{\nu}{2}+\frac{1}{2}\right)\right]^{-1}. \tag{39}$$



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)]

$$\Psi_\alpha^{(b)}(x_1, \ldots, x_N) = \Theta(x_1, \ldots, x_N)\Psi_\alpha^{(f)}(x_1, \ldots, x_N), \qquad (40)$$

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

$$\Psi_\alpha^{(f)}(x_1, \ldots, x_N) = (N!)^{-1/2} \det[\phi_{n_i}(x_j)]_{n_i \in \{n_1, \ldots, n_N\};\, x_j \in \{x_1, \ldots, x_N\}}. \qquad (41)$$

- The system constituted of strongly interacting bosons can be mapped into the ideal Fermi gas, whose ground-state many-body wave function yields

$$\Psi_0^{(b)}(x_1, \ldots, x_N) = \frac{2^{N(N-1)/4}}{a_0^{N/2}} \left(N! \prod_{n=0}^{N-1} n! \sqrt{\pi} \right)^{-1/2} \times \prod_{i=0}^{N} \mathrm{e}^{-x_i^2/2a_0^2} \prod_{1 \le j < k \le N} |x_k - x_j|. \qquad (42)$$

Finite T correlator

- The j-body correlator is given by

$$\varrho^{(j)}(x_1,\ldots,x_j;x_1',\ldots,x_j') = \frac{N!}{(N-j)!}\mathcal{Z}^{-1}\sum_{\alpha}\mathrm{e}^{-\beta E_\alpha}$$
$$\times\int_{\Re} dx_{j+1}\ldots dx_N \Psi_\alpha^{(b)*}(x_1,\ldots,x_N)\Psi_\alpha^{(b)}(x_1',\ldots,x_j',x_{j+1},\ldots,x_N). \tag{43}$$

- $\varrho^{(1)}$ of the bosonic system in terms of the fermionic wave function, yielding

$$\varrho^{(1)}(x,x') = \frac{N}{\mathcal{Z}}\sum_{\alpha}\mathrm{e}^{-\beta E_\alpha}\sum_{j=1}^{N-1}\binom{N-1}{j}(-2)^j[\mathrm{sgn}(x-x')]^j$$
$$\times\int_x^{x'} dx_2\ldots dx_{j+1}\int dx_{j+2}\ldots dx_N \Psi_\alpha^{(f)}(x,x_2,\ldots,x_N)\Psi_\alpha^{(f)}(x',x_2,\ldots,x_N). \tag{44}$$

Momentum distribution in the TG limit

- For small distances, it is possible to algebraically work out the last expression and approximate it by

$$\varrho^{(1)}(x,x') \approx \frac{|x'-x|^3}{2} F(R), \qquad R \equiv \frac{x+x'}{2}, \tag{45}$$

where

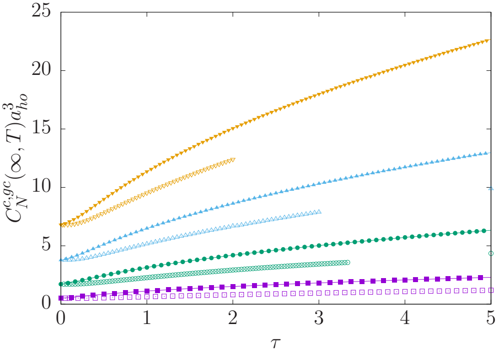
$$F(R) \equiv \mathcal{Z}^{-1} \sum_{n_1,n_2,\dots,n_N} \mathrm{e}^{-\beta \sum_{i=1}^{N} \epsilon_{n_i}}$$
$$\times \sum_{j\neq k} \left\{ \left[\phi_{n_j}(R)\partial_R \phi_{n_k}(R)\right]^2 - \phi_{n_j}(R)\phi_{n_k}(R)\partial_R\phi_{n_j}(R)\partial_R\phi_{n_k}(R) \right\}. \tag{46}$$

- From the momentum distribution $n(k) = \frac{1}{2\pi}\int dx \int dx' \, \mathrm{e}^{ik(x-x')}\varrho^{(1)}(x,x')$ and making use of the asymptotics of the Fourier transform $\int dx \, \mathrm{e}^{-ik(x-x_0)}|x-x_0|^{a-1} f(x) = \frac{2}{k^a} f(x_0)\cos(\pi a/2)\Gamma(a)$, and the definition of the contact $\mathcal{C} \equiv k^4 n(k)$ as $k \to \infty$ we get

$$\mathcal{C} = \frac{2}{\pi}\int_{-\infty}^{+\infty} dx \, F(x). \tag{47}$$

Tonks-Girardeau Tan's contact

$$
\begin{aligned}
\mathcal{C} = \frac{2}{\pi} \int dx\, \mathcal{Z}^{-1} \sum_{n_1, n_2, \ldots, n_N} \mathrm{e}^{-\beta \sum_{i=1}^{N} \epsilon_{n_i}} \\
\times \sum_{j \neq k} \left\{ \left[\phi_{n_j}(x) \partial_x \phi_{n_k}(x) \right]^2 - \phi_{n_j}(x) \phi_{n_k}(x) \partial_x \phi_{n_j}(x) \partial_x \phi_{n_k}(x) \right\}
\end{aligned}
\tag{48}
$$



arXiv:1908.08714, F.T.Sant'Ana, F. Hébert, V. Rousseau, M. Albert, P. Vignolo

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

$$f_N(\tilde{g}, T=0) \equiv \frac{\mathcal{C}_N(\tilde{g}, T=0)}{\mathcal{C}_N(\tilde{g} \to \infty, T=0)}, \tag{49}$$

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

$$f_N(\tilde{g}, T=0) \simeq f_2(\tilde{g}, T=0). \tag{50}$$

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

Large-temperature scaling

- For temperatures large enough, $\tau \gg 1$, 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,

$$\mathcal{C}_N(\tilde{g}, \tau \gg 1) = \frac{N(N-1)}{2} \mathcal{C}_2(\tilde{g}, \tau \gg 1). \tag{51}$$

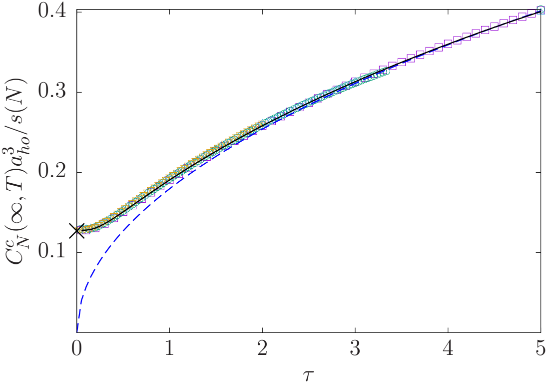
- Then, in the strongly interacting limit we find can extract all N dependence as

$$\mathcal{C}_N\left(\tilde{g} \to \infty, \tau \gg 1\right) = \frac{\sqrt{\tau}}{a_0^3 \pi^{3/2}} \left(N^{5/2} - N^{3/2}\right). \tag{52}$$

Generalized scaling conjecture in the TG limit

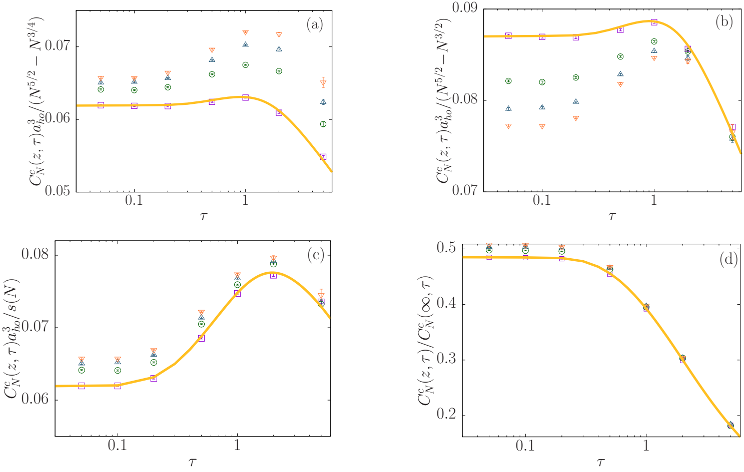
- Zero-temperature scaling: $\mathcal{C}_N(\tilde{g} \to \infty, \tau \ll 1) \propto N^{5/2} - N^{3/4}$
- Large-temperature scaling: $\mathcal{C}_N(\tilde{g} \to \infty, \tau \gg 1) \propto N^{5/2} - N^{3/2}$
- Generalized scaling conjecture:

$$\mathcal{C}_N(\tilde{g} \to \infty, \tau) \propto N^{5/2} - N^{3/4[1+\exp(-2/\tau)]} \tag{53}$$



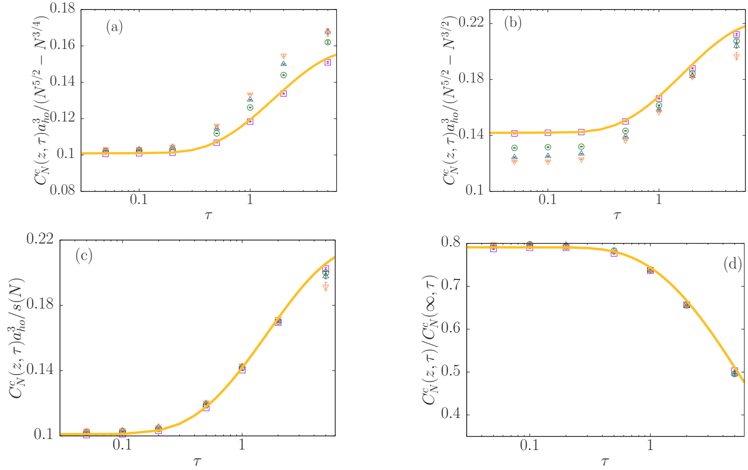
arXiv:1908.08714

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



arXiv:1908.08714

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



arXiv:1908.08714

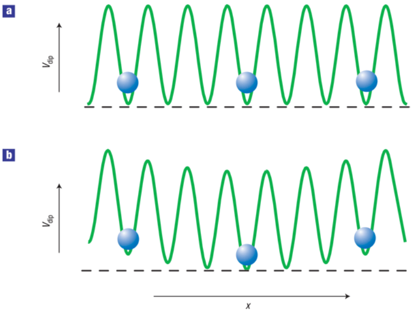
Conclusive remarks

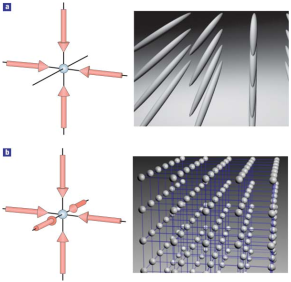
- We evaluated the contact for the harmonically trapped Tonks-Girardeau gas;
- We worked out a scaling factor for the contact in the TG limit for any temperature;
- Relying on QMC simulations, we showed that all previously stated scalings in the TG limit also apply for the finite interaction regime;
- 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 τ.

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)

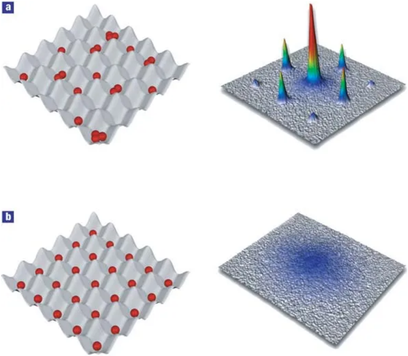
The Bose-Hubbard model

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

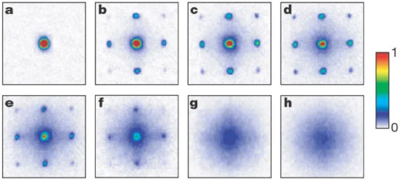
$$\hat{H}_{BH} = \frac{U}{2}\sum_{i} \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i - J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j - \mu \sum_{i} \hat{a}_i^\dagger \hat{a}_i. \tag{54}$$

- 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
- μ denotes the chemical potential

Phase transition



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



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

(a) For $J \gg U$ 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) For $U \gg J$ the system is in the Mott insulator phase: all atoms are localized in its respective potential minima with low momentum.

Mean-field approximation

From the Bose-Hubbard Hamiltonian

$$\hat{H}_{BH} = \frac{U}{2} \sum_i \left(\hat{n}_i^2 - \hat{n}_i \right) - \mu \sum_i \hat{n}_i - J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j, \tag{55}$$

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 Ψ is called *mean-field*;
2. Neglect quadratic terms of fluctuation, δ^2.

Such steps lead to the mean-field Hamiltonian,

$$\hat{H}_{MF} = \frac{U}{2} \sum_i \left(\hat{n}_i^2 - \hat{n}_i \right) - \sum_i \mu \hat{n}_i - Jz \sum_i \left(\Psi^* \hat{a}_i + \Psi \hat{a}_i^\dagger - \Psi^* \Psi \right). \tag{56}$$

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

$$\hat{H} = \frac{U}{2} \left(\hat{n}^2 - \hat{n} \right) - \mu \hat{n} - Jz \left(\Psi^* \hat{a} + \Psi \hat{a}^\dagger - \Psi^* \Psi \right). \tag{57}$$

Landau theory

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

$$\mathcal{F} = a_0 + a_2|\Psi|^2 + a_4|\Psi|^4 + \cdots . \tag{58}$$

- Extremizing it with respect to the order parameter

$$\frac{\partial \mathcal{F}}{\partial \Psi} = \Psi^* \left(a_2 + 2a_4|\Psi|^2\right) = 0, \tag{59}$$

the solutions are

$$\Psi = 0, \quad \text{(Mott insulator)} \tag{60a}$$

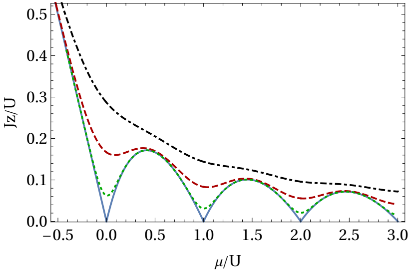
$$|\Psi|^2 = -\frac{a_2}{2a_4}. \quad \text{(Superfluid)} \tag{60b}$$

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

Phase diagram

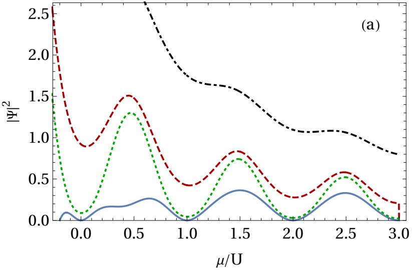
- Phase boundary:

$$a_2 = 0. \qquad (61)$$



- Condensate density:

$$|\Psi|^2 = -\frac{a_2}{2a_4}. \qquad (62)$$



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:

$$\begin{aligned} E_n &= E_{n+1} \\ \frac{U}{2}n(n-1) - \mu n &= \frac{U}{2}n(n+1) - \mu(n+1) \\ \frac{\mu}{U} &= n \end{aligned} \tag{63}$$

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

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

$$\hat{\mathcal{P}} + \hat{\mathcal{Q}} = \hat{\mathbb{1}}. \tag{64}$$

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

$$\hat{\mathcal{P}} \left[\hat{H} + \lambda \hat{V} \hat{\mathcal{Q}} \left(E_n - \hat{\mathcal{Q}} \hat{H} \hat{\mathcal{Q}} \right)^{-1} \hat{\mathcal{Q}} \lambda \hat{V} \right] \hat{\mathcal{P}} |\Psi_n\rangle = E_n \hat{\mathcal{P}} |\Psi_n\rangle, \tag{65}$$

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

$$\hat{\mathcal{P}}\hat{H}_{\text{eff}}\hat{P}|\Psi_n\rangle = E_n\hat{\mathcal{P}}|\Psi_n\rangle, \tag{66}$$

with

$$\hat{H}_{\text{eff}} \equiv \hat{H} + \lambda^2\hat{V}\hat{\mathcal{Q}}\left(E_n - \hat{\mathcal{Q}}\hat{H}\hat{\mathcal{Q}}\right)^{-1}\hat{\mathcal{Q}}\hat{V}. \tag{67}$$

- The effective Hamiltonian can then be expanded in series with respect to λ:

$$\begin{aligned}\hat{H}_{\text{eff}} =& \hat{H}_0 + \lambda\hat{V} + \lambda^2\sum_{l\in\mathcal{Q}}\frac{\hat{V}|\Psi_l^{(0)}\rangle\langle\Psi_l^{(0)}|\hat{V}}{E_n - E_l^{(0)}} \\ &+ \lambda^3\sum_{l,l'\in\mathcal{Q}}\frac{\hat{V}|\Psi_l^{(0)}\rangle\langle\Psi_l^{(0)}|\hat{V}|\Psi_{l'}^{(0)}\rangle\langle\Psi_{l'}^{(0)}|\hat{V}}{\left(E_n - E_l^{(0)}\right)\left(E_n - E_{l'}^{(0)}\right)} \\ &+ \lambda^4\sum_{l,l',l''\in\mathcal{Q}}\frac{\hat{V}|\Psi_l^{(0)}\rangle\langle\Psi_l^{(0)}|\hat{V}|\Psi_{l'}^{(0)}\rangle\langle\Psi_{l'}^{(0)}|\hat{V}|\Psi_{l''}^{(0)}\rangle\langle\Psi_{l''}^{(0)}|\hat{V}}{\left(E_n - E_l^{(0)}\right)\left(E_n - E_{l'}^{(0)}\right)\left(E_n - E_{l''}^{(0)}\right)} \\ &+ \cdots.\end{aligned} \tag{68}$$

One-state approach

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

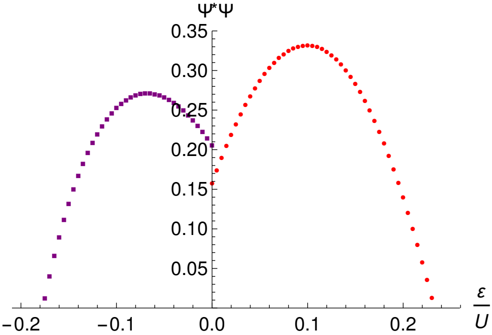
$$\hat{\mathcal{P}} = |n\rangle\langle n|. \tag{69}$$

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

$$\begin{aligned} E_n =& E_n^{(0)} + \lambda J z \Psi^* \Psi + \lambda^2 J^2 z^2 \Psi^* \Psi \left(\frac{n}{E_n - E_{n-1}^{(0)}} + \frac{n+1}{E_n - E_{n+1}^{(0)}} \right) \\ &+ \lambda^3 J^3 z^3 \left(\Psi^* \Psi\right)^2 \left[\frac{n}{\left(E_n - E_{n-1}^{(0)}\right)^2} + \frac{n+1}{\left(E_n - E_{n+1}^{(0)}\right)^2} \right] + \cdots . \end{aligned} \tag{70}$$

Condensate density

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



M. Kübler, F.T. Sant'Ana, F.E.A. dos Santos, A. Pelster, *Phys. Rev. A* **99**, 063603 (2019)

Two-state approach

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

$$\hat{\mathcal{P}} = |n\rangle\langle n| + |n+1\rangle\langle n+1|. \tag{71}$$

- Now we have a determinantal equation for the energy

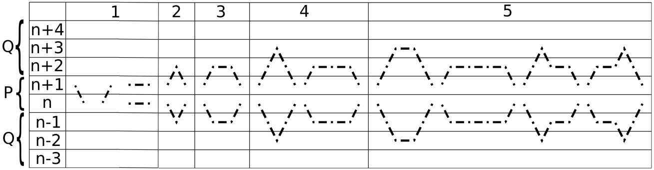
$$\begin{vmatrix} H_{\mathrm{eff},n,n} - E_n & H_{\mathrm{eff},n,n+1} \\ H_{\mathrm{eff},n+1,n} & H_{\mathrm{eff},n+1,n+1} - E_n \end{vmatrix} = 0. \tag{72}$$

- We can extract physical quantites from

$$\det\left(\Gamma - \mathbb{I}E_n\right) = 0, \tag{73a}$$

$$\frac{1}{\Psi}\frac{\partial\left|\Gamma - \mathbb{I}E_n\right|}{\partial\Psi^*} = 0, \tag{73b}$$

Graphical approach



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- Starting point:

$$S\,(m) = E_n - E_m^{(0)}. \tag{74}$$

- Ascending lines:

$$L_A\,(m) = -\lambda J z \Psi \frac{\sqrt{m+1}}{E_n - E_m^{(0)}}. \tag{75}$$

- Descending lines:

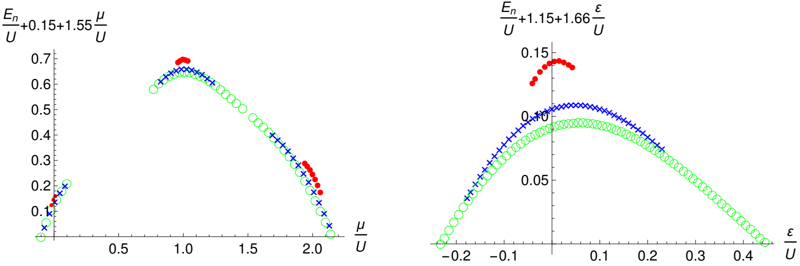
$$L_D\,(m) = -\lambda J z \Psi^* \frac{\sqrt{m}}{E_n - E_m^{(0)}}. \tag{76}$$

- Horizontal lines:

$$L_H(m) = \frac{\lambda J z \Psi^* \Psi}{E_n - E_m^{(0)}}. \tag{77}$$

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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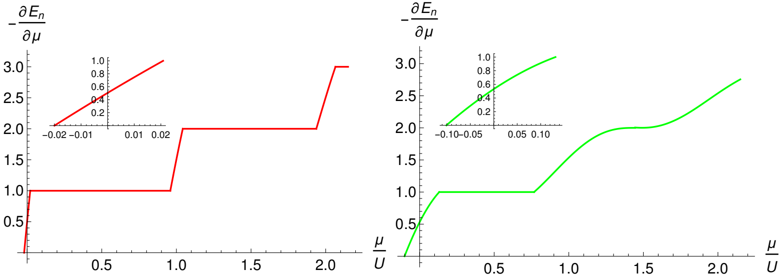
Particle density at T=0

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



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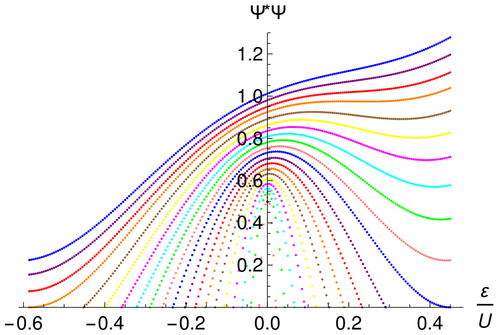
Zero-temperature condensate density

- Condensate densities $\Psi^*\Psi$ as functions of $\varepsilon/U = \mu/U - n$ for $n = 1$ up to λ^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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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

$$\hat{\mathcal{P}} = |n\rangle\langle n| + |n+1\rangle\langle n+1|, \tag{78}$$

$$\hat{\mathcal{Q}} = \sum_{m \notin \mathcal{P}} |m\rangle\langle m|. \tag{79}$$

- Adding the operators:

$$\hat{H} = \hat{H}_0 + \left(\hat{\mathcal{P}} + \hat{\mathcal{Q}}\right) \hat{V} \left(\hat{\mathcal{P}} + \hat{\mathcal{Q}}\right). \tag{80}$$

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

$$\hat{\mathcal{H}}_0 \equiv \hat{H}_0 + \hat{\mathcal{P}}\hat{V}\hat{\mathcal{P}}, \tag{81a}$$

$$\hat{\mathcal{V}} \equiv \hat{\mathcal{P}}\hat{V}\hat{\mathcal{Q}} + \hat{\mathcal{Q}}\hat{V}\hat{\mathcal{P}} + \hat{\mathcal{Q}}\hat{V}\hat{\mathcal{Q}}. \tag{81b}$$

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

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

$$\mathcal{E}_\pm = \frac{E_n + E_{n+1}}{2} \pm \frac{1}{2}\sqrt{\left(E_n - E_{n+1}\right)^2 + 4J^2 z^2 |\Psi|^2 \left(n+1\right)}. \tag{82}$$

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

$$|\Phi_\pm\rangle = \frac{1}{\sqrt{1 + \frac{|\mathcal{E}_\pm - E_n|^2}{J^2 z^2 |\Psi|^2 (n+1)}}} \left[|n\rangle + \frac{E_n - \mathcal{E}_\pm}{Jz\sqrt{|\Psi|^2 \left(n+1\right)}} |n+1\rangle \right]. \tag{83}$$

Time-dependent perturbation theory

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

$$\frac{d\hat{\mathcal{U}}_{\mathrm{I}}(\tau)}{d\tau} = -\hat{\mathcal{V}}_{\mathrm{I}}(\tau)\hat{\mathcal{U}}_{\mathrm{I}}(\tau). \tag{84}$$

2. Dyson series:

$$\hat{\mathcal{U}}_{\mathrm{I}}(\beta) \approx \hat{\mathcal{U}}_{\mathrm{I}}(0) - \int_0^\beta d\tau_1 \hat{\mathcal{V}}_{\mathrm{I}}(\tau_1) + \int_0^\beta d\tau_1 \int_0^{\tau_1} d\tau_2 \hat{\mathcal{V}}_{\mathrm{I}}(\tau_1)\hat{\mathcal{V}}_{\mathrm{I}}(\tau_2). \tag{85}$$

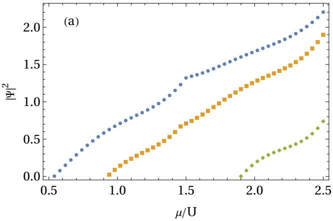
3. Goal:

$$\mathcal{F} = -\frac{1}{\beta}\log\left(\mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{\mathcal{H}}_0}\hat{\mathcal{U}}_{\mathrm{I}}(\beta)\right]\right). \tag{86}$$

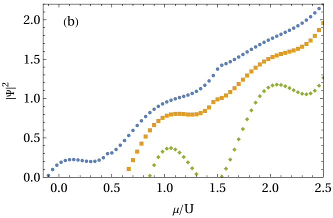
4. Condensate density:

$$\frac{\partial\mathcal{F}}{\partial|\Psi|^2} = 0. \tag{87}$$

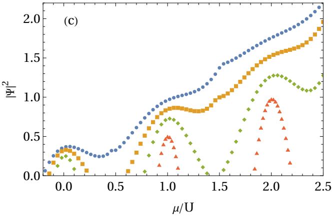
Condensate densities



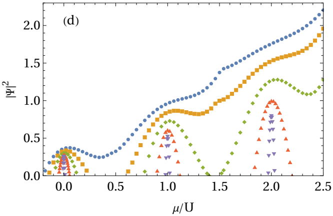
(a) $\beta = 5/U$



(b) $\beta = 10/U$



(c) $\beta = 30/U$



(d) $\beta \to \infty$

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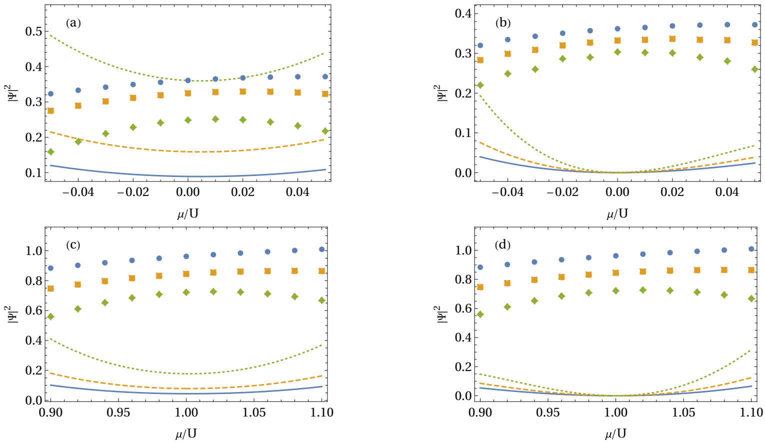
Comparison between NDPT and FTDPT



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

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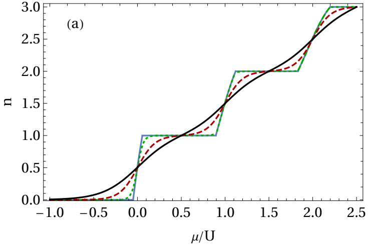
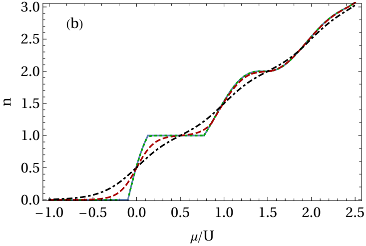
Particle density

- 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 developed 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 in a wide range of optical-lattice systems that presents similar Mott-lobe structures.

Thank you!