Upper Bound on the Condensate in Hard Core Bose Lattice Gas

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Abstract. Using methods developed by G. Roepstorf we prove upper bound for the amount of condensate in *hard core* Bose lattice gas.

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1. Introduction

In [4] Roepstorff proved the following inequality:

$$\langle A^* A \rangle \geq \langle [A, A^*] \rangle \left\{ \exp \frac{\beta \langle [C^*, [H, C]] \rangle \langle [A, A^*] \rangle}{|\langle [A, C^*] \rangle|^2} - 1 \right\}^{-1} \tag{1.1}$$

where $\langle \cdots \rangle$ stands for thermal expectation:

$$\langle A \rangle = \frac{\mathrm{Tr}\left(e^{-\beta H} A\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} \tag{1.2}$$

and A and C are any two bounded operators. In a second paper, [5], the same author used this inequality to prove an upper bound on the amount of condensate for a Bose gas in $\mathbf{R}^d$, $d \geq 3$, with arbitrary pair interaction.

Exploiting the same methods we give an upper bound for the amount of condensate for a *hard core* Bose lattice gas. As, due to the hard core condition, the commutation relations of the emerging creation and annihilation operators are different of the standard bosonic ones, this upper bound is better than that proved by Roepstorff, and reflects the $\rho \leftrightarrow 1-\rho$ symmetry of the condensation in this model. (See the remarks after Proposition 1.)

This result is an adaptations of Roepstorff's method, we don't claim any originality of the ideas. Nevertheless, as condensation of the hard core Bose lattice gas is an intriguing open problem, we think that this applications is worth mentioning.

2. The Upper Bound

We consider a Bose lattice gas on $\mathbf{Z}^d$, or on a d-dimensional discrete torus Λ, interacting via a pair potential which has a hard core, otherwise arbitrary. The local creation and annihilation operators $a^+(x),\ a(x):\ x \in \mathbf{Z}^d$ satisfy the following commutation relations:

$$[a(x), a(y)] = [a^+(x), a^+(y)] = 0, \ \ [a(x), a^+(y)] = \delta_{x,y}\big(1 - 2n(x)\big). \tag{2.1}$$

where the local occupation number operator is

$$n(x) = a^+(x) a(x) = \big[n(x)\big]^2. \tag{2.2}$$

The Hamiltonian of our Bose gas is

$$H_0 = -\frac{1}{2} \sum_{\langle x,y \rangle} a^+(x) a(y) + \frac{1}{2} \sum_{x,y \in \Lambda} V(x-y) n(x) n(y) + \mu \sum_{x \in \Lambda} n(x). \tag{2.3}$$

Where the first sum extends over neighbouring sites and periodic boundary conditions are considered.

We denote the density of the gas by ρ, $\rho = \langle a^+(x)a(x)\rangle$. The amount of condensate (i.e. the order parameter of Bose-Einstein condensation) is defined cf. ref. [1] as

$$\rho_c = \lim_{\Lambda \nearrow \mathbf{Z}^d} \frac{1}{|\Lambda|^2} \sum_{x,y\in\Lambda} \langle a^+(x)a(y)\rangle \tag{2.4}$$

We prove the following upper bound for the amount of condensate:

Proposition 1. *In three and more dimensions*

$$\rho_c(\rho,\beta) \leq \min\left\{x(\rho,\beta)\,,\, \rho(1-\rho)\right\} \tag{2.5}$$

where $x(\rho,\beta)$ *is the unique solution of the equation*

$$x = \frac{1}{2} - \left(\frac{1}{2} - \rho\right) \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \coth \frac{\beta\left(\frac{1}{2}-\rho\right)\min\{\rho\,,\,1-\rho\}D(\mathbf{p})}{x} d\mathbf{p} \tag{2.6}$$

and

$$D(\mathbf{p}) = \sum_{i=1}^{d} (1-\cos p_i) \tag{2.7}$$

Remarks. (1) As in 1 and 2 dimensions the equation (2.6) has no positive solution, the theorem of Mermin and Wagner is recovered: in less than three dimensions there is no Bose-Einstein condensation in these models.
(2) For the sake of comparison: the upper bound proved in [5], applied to the lattice gas case would result in a similar Proposition, with $x(\rho,\beta)$ being the unique solution of the equation

$$x = \rho - \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \left\{\exp\frac{\beta\rho D(\mathbf{p})}{x} - 1\right\}^{-1} d\mathbf{p} \tag{2.8}$$

Roepstorff's upper bound is completely independent of the interaction. In our derivation the hard core is taken into account, hence the improvement.
(3) Apart from being somewhat stronger, our upper bound has the advatage of showing the same symmetry as the condensate itself:

$$\rho_c(\rho,\beta) = \rho_c(1-\rho,\beta) \qquad \text{and} \qquad x(\rho,\beta) = x(1-\rho,\beta) \tag{2.9}$$

Proof. We apply Roepstorff's inequality with the following choices of the operators:

$$H_\varepsilon = H_0 - \frac{\varepsilon}{2}\sum_{x\in\Lambda}\left(a^+(x) + a(x)\right) \tag{2.10}$$

with periodic boundary conditions on the discrete torus Λ. Note that a symmetry breaking term is added to the Hamiltonian (2.3). $\langle\cdots\rangle_{\Lambda,\varepsilon}$ will denote thermal expectation with respect to this Hamiltonian.

$$A = \hat{a}(\mathbf{p}) = \sum_{x\in\Lambda} e^{i\mathbf{p}\cdot x} a(x), \quad A^* = \hat{a}^+(-\mathbf{p}) = \sum_{x\in\Lambda} e^{-i\mathbf{p}\cdot x} a^+(x), \tag{2.11}$$

$$C = \hat{n}(\mathbf{p}) = \sum_{x\in\Lambda} e^{i\mathbf{p}\cdot x} n(x), \quad C^* = \hat{n}(-\mathbf{p}) = \sum_{x\in\Lambda} e^{-i\mathbf{p}\cdot x} n(x), \tag{2.12}$$

$$\mathbf{p} \in \Lambda^* \subset [-\pi,\pi]^d.$$

The commutators appearing in (1.1) will be

$$[A, A^*] = \big[\hat{a}(\mathbf{p}), \hat{a}^+(-\mathbf{p})\big] = |\Lambda| - 2\sum_{x\in\Lambda} n(x), \tag{2.13}$$

$$[A, C^*] = [\hat{a}(\mathbf{p}), \hat{n}(-\mathbf{p})] = \sum_{x\in\Lambda} a(x), \tag{2.14}$$

$$[C,[H,C^*]] = [\hat{n}(\mathbf{p}), [H_\varepsilon, \hat{n}(-\mathbf{p})]] =$$

$$\sum_{x\in\Lambda}\left\{\sum_{\delta\in\Lambda,|\delta|=1} (1-\cos\mathbf{p}\cdot\delta)\, a^+(x)a(x+\delta) + \frac{\varepsilon}{2}\left(a^+(x)+a(x)\right)\right\}. \tag{2.15}$$

And the corresponding expectations:

$$\langle[A,A^*]\rangle = \left\langle\big[\hat{a}(\mathbf{p}), \hat{a}^+(-\mathbf{p})\big]\right\rangle_{\Lambda,\varepsilon} = |\Lambda|\left(1 - 2\langle n(0)\rangle_{\Lambda,\varepsilon}\right), \tag{2.16}$$

$$\langle[A,C^*]\rangle = \langle[\hat{a}(\mathbf{p}), \hat{n}(-\mathbf{p})]\rangle_{\Lambda,\varepsilon} = |\Lambda|\langle a(0)\rangle_{\Lambda,\varepsilon}, \tag{2.17}$$

$$\langle[C,[H,C^*]]\rangle = \langle[\hat{n}(\mathbf{p}), [H_\varepsilon, \hat{n}(-\mathbf{p})]]\rangle_{\Lambda,\varepsilon} =$$

$$|\Lambda|\left\{\sum_{\delta\in\Lambda,|\delta|=1} (1-\cos\mathbf{p}\cdot\delta)\left\langle a^+(0)a(\delta)\right\rangle_{\Lambda,\varepsilon} + \varepsilon\langle a(0)\rangle_{\Lambda,\varepsilon}\right\}. \tag{2.18}$$

We use the inequality

$$\begin{aligned}\left\langle a^+(0)a(\delta)\right\rangle_{\Lambda,\varepsilon} &\le \min\left\{\left\langle a^+(0)a(0)\right\rangle_{\Lambda,\varepsilon}, \left\langle a(0)a^+(0)\right\rangle_{\Lambda,\varepsilon}\right\} \\ &= \min\left\{\langle n(0)\rangle_{\Lambda,\varepsilon}, 1-\langle n(0)\rangle_{\Lambda,\varepsilon}\right\}\end{aligned} \tag{2.19}$$

to get

$$\langle[C,[H,C^*]]\rangle \le |\Lambda|\left(D(\mathbf{p})\min\left\{\langle n(0)\rangle_{\Lambda,\varepsilon}, 1-\langle n(0)\rangle_{\Lambda,\varepsilon}\right\} + \varepsilon\langle a(0)\rangle_{\Lambda,\varepsilon}\right). \tag{2.20}$$

Pluging all these in (1.1) we get

$$|\Lambda|^{-1}\big\langle \hat{a}^+(-\mathbf{p})\hat{a}(\mathbf{p})\big\rangle_{\Lambda,\varepsilon} \geq$$

$$\Big(1-2\langle n(0)\rangle_{\Lambda,\varepsilon}\Big)\left\{\exp\frac{\beta\Big(D(\mathbf{p})\min\Big\{\langle n(0)\rangle_{\Lambda,\varepsilon}\,,\,1-\langle n(0)\rangle_{\Lambda,\varepsilon}\Big\}+\varepsilon\langle a(0)\rangle_{\Lambda,\varepsilon}\Big)\Big(1-2\langle n(0)\rangle_{\Lambda,\varepsilon}\Big)}{\langle a(0)\rangle^2_{\Lambda,\varepsilon}}-1\right\}^{-1} \tag{2.21}$$

And now taking the limits $\Lambda \nearrow \mathbf{Z}^d$, $\varepsilon \searrow 0$ and integrating over the cube $[-\pi,\pi]^d$ (in this order!) leads us to the inequality

$$\rho-\bar{\rho}_c \geq (1-2\rho)\,\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}\left\{\exp\frac{\beta D(\mathbf{p})\min\{\rho\,,\,1-\rho\}\,(1-2\rho)}{\eta^2}-1\right\}^{-1}d\mathbf{p}. \tag{2.22}$$

Where

$$\eta = \lim_{\varepsilon\searrow 0}\lim_{\Lambda\nearrow\mathbf{Z}^d}\langle a(0)\rangle_{\Lambda,\varepsilon} \tag{2.23}$$

$$\bar{\rho}_c = \lim_{\varepsilon\searrow 0}\lim_{\Lambda\nearrow\mathbf{Z}^d}\frac{1}{|\Lambda|^2}\sum_{x,y\in\Lambda}\big\langle a^+(x)a(y)\big\rangle_{\Lambda,\varepsilon} \tag{2.24}$$

(Alternatively, one can get (2.22) by summing over $\mathbf{p}\neq 0$ in (2.21) and then taking the limit $\Lambda\nearrow\mathbf{Z}^d$.) Using the inequalities

$$\rho_c \leq \eta^2 \leq \bar{\rho}_c, \tag{2.25}$$

(the first one of which is proved in the last section of [5], the second one is trivial) we arrive to

$$\rho_c \leq x(\rho,\beta) \tag{2.26}$$

as given in (2.6). As mentioned in ref. [3], the bound

$$\rho_c \leq \rho(1-\rho) \tag{2.27}$$

easily follows from the method of ref. [2], applied to the hard core Bose lattice gas case. We don't repeat here that argument.

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