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A Remark on the Condensation in the Hard-Core Lattice Bose Gas

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We point out that Bose–Einstein condensation occurs at sufficiently low temperature in a hard-core $\mathbb{Z}^d$-lattice Bose gas for $d \geqslant 3$ and particle density 1/2, by exploiting its equivalence to a spin-1/2 XY model.

KEY WORDS: Lattice Bose gas; hard-core interaction; Bose–Einstein condensation.

1. The study of lattice Bose gas models was proposed[1] in an attempt to understand the effect of the interaction on Bose–Einstein condensation. It was shown in ref. 1 that, if the interaction has a hard core (i.e., each site could be occupied by at most one particle), then the model can be represented as a quantum spin-1/2 model on the given lattice. The approximate study of the phase diagram by mean-field and spin-wave techniques was hence possible.

Recently, the exact solution, exhibiting condensation, for the hard-core (h.c.) Bose gas on a complete graph has been obtained.[2,3] The one-particle operator in this model is, however, dependent on the number of sites and has no proper spatial structure; in spin language it corresponds to the mean-field XY model. These papers revived the interest in a rigorous study of the more realistic model of the h.c. Bose gas on the $\mathbb{Z}^d$-graph with edges between nearest neighbors as initially proposed in ref. 1. In a recent paper Toth[4] derives, by adapting Roepstorff's method[5] to the h.c. situation, an improved upper bound on the condensate. Efforts have also been made toward obtaining an exact solution of the model on different graphs.[6]

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In this note we point out that, insofar as one is interested only in establishing condensation, a straightforward application of the Gaussian domination argument of ref. 7 is sufficient to prove it in the h.c. Bose gas on the $\mathbb{Z}^d$-graph at low temperature in a half-filled $\mathbb{Z}^d$-lattice for $d \geqslant 3$. Unfortunately, the argument breaks down for other densities. To give support to the conjecture that condensation persists in a whole density range around 1/2, we show that this is the case for a "classical limit" of the model: the classical XY model in a tranverse field.

2. We shall define the h.c. Bose gas model on $\mathbb{Z}^d$ and rederive its representation as a spin-1/2 XY model. Bose condensation in the former turns out to be equivalent to ferromagnetic long-range order in the latter.

Let $\Lambda = \{x \in \mathbb{Z}^d : 0 \leqslant x^i < N,\quad i = 1,..., d\}$. The one-particle Hilbert space is $\mathscr{H}_\Lambda = \mathbb{C}^\Lambda$ with the canonical basis $\{e_x : x \in \Lambda\}$, with $e_x(y) = \delta_{xy}$ representing the state with one particle at site $x \in \Lambda$. The one-particle kinetic energy operator $\mathscr{k}_\Lambda$ is taken to be

$$(\mathscr{k}_\Lambda \phi)(x) = -(1/2)\, \Delta\phi(x) = (1/2) \sum_{y \in \Lambda, \langle y, x\rangle} [\phi(x) - \phi(y)] \tag{1}$$

where $\phi = \sum_{x \in \Lambda} \phi(x)\, e_x \in \mathscr{H}_\Lambda$ and $\langle y, x\rangle$ means that x, y are nearest neighbours (n.n.) on the torus Λ (periodic boundary conditions). The eigenvalues and eigenvectors of $\mathscr{k}_\Lambda$ are

$$\varepsilon_k = 2 \sum_{j=1}^{d} \sin^2(k^j/2); \qquad \phi_k(x) = N^{-d/2} e^{ikx} \tag{2}$$

where $k \in B_\Lambda := [(2\pi/N)\{0,..., N-1\}]^d$. Let $\mathscr{F}_\Lambda$ be the symmetric Fock space over $\mathscr{H}_\Lambda$ and b_x^* (b_x) and $\hat{b}_k^*$ ($\hat{b}_k$) be the usual creation (annihilation) operators on $\mathscr{F}_\Lambda$ corresponding to e_x and ϕ_k, respectively. The number operator and free Hamiltonian are therefore

$$N_\Lambda = \sum_{x \in \Lambda} b_x^* b_x \tag{3}$$

$$H_\Lambda^0 = (1/2) \sum_{\langle x, y\rangle} (b_x^* - b_y^*)(b_x - b_y) = \sum_{k \in \Lambda} \varepsilon_k \hat{b}_k^* \hat{b}_k \tag{4}$$

Here $\sum_{\langle x, y\rangle}$ means summation over the (unordered) pairs of n.n. in Λ. The thermodynamics of the free lattice gas is hence obtained as usual.

To switch on the hard-core interaction means to discard all states with more than one particle at one site, i.e., to restrict everything to the subspace $\mathscr{F}_\Lambda^{\mathrm{hc}}$ of $\mathscr{F}_\Lambda$ spanned by the orthonormal vectors:

$$\Psi_X = \prod_{x \in X} b_x^* \,|0\rangle, \qquad X \subset \Lambda$$

With P denoting the orthogonal projection onto $\mathscr{F}_\Lambda^{\rm hc}$, let us define

$$a_x = Pb_x|_{\mathscr{F}_\Lambda^{\rm hc}} \tag{5}$$

Because $b_x \mathscr{F}_\Lambda^{\rm hc} \subset \mathscr{F}_\Lambda^{\rm hc}$,

$$a_x = b_x|_{\mathscr{F}_\Lambda^{\rm hc}}$$

One can easily check that its adjoint is

$$a_x^* = Pb_x^*|_{\mathscr{F}_\Lambda^{\rm hc}}$$

The major difference between $a_x^{(*)}$ and $b_x^{(*)}$ consists in their different commutation properties: $[a_x^{(*)}, a_y^{(*)}] = 0$ for $x \neq y$, but $a_x^2 = a_x^{*2} = 0$, $a_x a_x^* + a_x^* a_x = \mathrm{I}$. For every operator A on $\mathscr{F}_\Lambda$ which is a monomial in b_x^* and b_x in normal form, the operation

$$PA|_{\mathscr{F}_\Lambda^{\rm hc}}$$

is equivalent to replacing all $b^{(*)}$ by $a^{(*)}$, e.g.,

$$PN_\Lambda|_{\mathscr{F}_\Lambda^{\rm hc}} = \sum_{x \in \Lambda} a_x^* a_x$$

which in fact equals

$$N_\Lambda|_{\mathscr{F}_\Lambda^{\rm hc}}$$

The Hamiltonian of the h.c. model is given by

$$H_\Lambda = (1/2) \sum_{\langle x, y \rangle} (a_x^* - a_y^*)(a_x - a_y) = \sum_{k \in B_\Lambda} \varepsilon_k \hat{a}_k^* \hat{a}_k = PH_\Lambda^0|_{\mathscr{F}_\Lambda^{\rm hc}} \tag{4'}$$

The Gibbs state will be

$$\langle \cdot \rangle_{\beta, \mu, \Lambda} = Z_\Lambda(\beta, \mu)^{-1} \operatorname{Tr}(\cdot \exp[-\beta(H_\Lambda - \mu N_\Lambda)])$$

where the trace is taken over $\mathscr{F}_\Lambda^{\rm hc}$, and $Z_\Lambda(\beta, \mu)$ is the normalizing factor: $\langle I \rangle_{\beta, \mu, \Lambda} = 1$.

We shall next consider the XY representation. For $x \in \Lambda$, let $(\mathbb{C}^2)_x$ be a two-dimensional space with orthonormal basis $\{|\sigma\rangle_x;\ \sigma = \pm 1/2\}$ and carrying the usual representation of the $\mathfrak{su}(2)$ algebra by Pauli matrices:

$$S_x^1 = \begin{pmatrix} 0 & 1/2 \\ 1/2 & 0 \end{pmatrix}, \quad S_x^2 = \begin{pmatrix} 0 & -i/2 \\ i/2 & 0 \end{pmatrix}, \quad S_x^3 = \begin{pmatrix} 1/2 & 0 \\ 0 & -1/2 \end{pmatrix}$$

Let

$$\mathscr{G}_\Lambda = \bigotimes_{x \in \Lambda} (\mathbb{C}^2)_x$$

A unitary $U: \mathscr{F}_\Lambda^{\text{hc}} \to \mathscr{G}_\Lambda$ is defined by

$$\Psi_X \overset{U}{\longmapsto} \bigotimes_{x \in \Lambda} |\sigma_X(x)\rangle_x$$

where $\sigma_X(x) = 1/2$ if $x \in X$ and $= -1/2$ if $x \in \Lambda \backslash X$. Then, one has

$$U a_x U^* = S_x^- = S_x^1 - iS_x^2 \tag{6}$$

by means of which one can make the translation of the model from $\mathscr{F}_\Lambda^{\text{hc}}$ to $\mathscr{G}_\Lambda$. In particular,

$$H_\Lambda^{\text{sp}} = U(H_\Lambda - \mu N_\Lambda)\, U^* = -\sum_{\langle x, y\rangle} (S_x^1 S_y^1 + S_x^2 S_y^2) - (\mu - d) \sum_{x \in \Lambda} (S_x^3 + \tfrac{1}{2} N^d) \tag{7}$$

which is, up to an irrelevant constant, the Hamiltonian of a spin-1/2 XY ferromagnet with exchange $J = 1$ in a transverse field $H = \mu - d$. We denote by $\langle \cdot \rangle_{\beta, H, \Lambda}^{\text{sp}}$ the corresponding Gibbs state on $\mathscr{G}_\Lambda$

Defining as usual the condensate density by

$$\rho_c(\beta, \mu) = \lim_{N \to \infty} N^{-d} \langle \hat{b}_0^* \hat{b}_0 \rangle_{\beta, \mu, \Lambda} = \lim_{N \to \infty} N^{-d} \langle \hat{a}_0^* \hat{a}_0 \rangle_{\beta, \mu, \Lambda} \tag{8}$$

our assertion is the following:

Proposition. For $d \geqslant 3$, $\mu = d$, and β sufficiently large, the h.c. Bose gas on $\mathbb{Z}^d$ has nonzero condensate density: $\rho_c(\beta, d) > 0$. The corresponding particle density is $\rho = \lim_{N \to \infty} N^{-d} \langle N_\Lambda \rangle_{\beta, d, \Lambda} = 1/2$.

Indeed, using (6) one obtains

$$\rho_c(\beta, \mu) = \lim_{N \to \infty} \left\langle \sum_{j=1}^{2} \left(N^{-d} \sum_{x \in \Lambda} S_x^j \right)^2 \right\rangle_{\beta, \mu - d, \Lambda}^{\text{sp}} \tag{9}$$

$$\rho(\beta, \mu) = 1/2 + \lim_{N \to \infty} \langle S_x^3 \rangle_{\beta, \mu - d, \Lambda}^{\text{sp}} \tag{10}$$

For $\mu = d$, the external field in (7) vanishes and one is exactly in the framework of Theorem 5.2 in ref. 7, which proves $\rho_c(\beta, d) > 0$ for large β. Also, $\langle S_x^3 \rangle_{\beta, 0, \Lambda}^{\text{sp}} = 0$ by symmetry, and $\rho = 1/2$.

3. If $\mu \neq d$, the approach of ref. 7 does not work, because their basic bound (Lemma 4.1) needs a real matrix representation of all S_x^i, $i = 1, 2, 3$. For the Ising ferromagnet on $\mathbb{Z}^d$ with $d \geqslant 2$ (where this is possible), Kirkwood[8] proved that long-range order is not destroyed by switching a small transverse field. It is to be expected that the XY model shares the same property. This agrees with physical intuition: a field orthogonal to the plane in which symmetry breaking occurs should not affect drastically the order parameter. We shall show below that this is true for its classical limit, which is relevant for high spin values. Though there is no hope to obtain in this way a proof for the h.c. Bose gas, which is the spin-1/2 case, the result may increase the confidence in such an expectation. The classical model is described as follows.

At every $x \in \Lambda$ lives a unit 3-dimensional vector $s_x = (s_x^1, s_x^2, s_x^3) \in \mathbf{S}^2$. Here $\mathbf{S}^2$ is endowed with the invariant measure ν. Consider the interaction Hamiltonian ($\mathbf{s} = \{s_x; x \in \Lambda\}$)

$$H_\Lambda^{\mathrm{cl}}(\mathbf{s}) = -\sum_{\langle x, y\rangle} (s_x^1 s_y^1 + s_x^2 s_y^2) - h \sum_{x \in \Lambda} s_x^3 \tag{11}$$

and denote $\langle\cdot\rangle_{\beta,h,\Lambda}^{\mathrm{cl}}$ the corresponding Gibbs measure.

We shall prove long-range order in this model, i.e.,

$$\lim_{N\to\infty} \left\langle \sum_{j=1}^{2} \left(N^{-d} \sum_{x\in\Lambda} s_x^j\right)^2 \right\rangle_{\beta,h,\Lambda}^{\mathrm{cl}} > 0 \tag{12}$$

for $|h| < h_0$ and $\beta > \beta_0(h)$. This follows, in an infrared bound approach,[9] from two basic bounds:

(i) For all $k \in B_\Lambda$, $k \neq 0$,

$$\sum_{j=1}^{2} \langle \hat{s}_k^j \hat{s}_{-k}^j \rangle_{\beta,h,\Lambda}^{\mathrm{cl}} \leqslant (\beta\varepsilon_k)^{-1}$$

with ε_k defined in Eq. (2).

(ii) There exists $h_0 > 0$ such that for $|h| < h_0$ one can find $\sigma > 0$ and $\beta_1 < \infty$, such that

$$\sum_{j=1}^{2} \langle (s_x^j)^2 \rangle_{\beta,h,\Lambda}^{\mathrm{cl}} \geqslant \sigma \qquad \text{for all} \quad \Lambda \quad \text{and} \quad \beta \geqslant \beta_1$$

Inequality (i) is the standard infrared bound, whose proof[9] is not affected by the external field. To show (ii), we start by finding the ground configurations. With $\rho_x = [(s_x^1)^2 + (s_x^2)^2]^{1/2}$, one has

$$H_{\Lambda}^{\mathrm{cl}}(\mathbf{s}) \geqslant -\sum_{\langle x, y \rangle} \rho_x \rho_y - |h| \sum_x (1-\rho_x^2)^{1/2}$$
$$\geqslant -\sum_x (d\rho_x^2 + |h|(1-\rho_x^2)^{1/2}) \geqslant -E_0 N^d \tag{13}$$

where $E_0 = d + (h^2/4d)$, with equalities iff all s_x are parallel, $s_x^3 h > 0$ and $\rho_x^2 = 1 - (h/2d)^2 := \rho^{*2}$ if $|h| < h_0 := 2d$, and $E_0 = |h|$ attained at $\rho_x = 0$ if $|h| \geqslant h_0$. Let now $\chi_{\sigma,x}$ be the characteristic function of $\mathbf{s} \in (\mathbf{S}^2)^{\Lambda}$ for which $\rho_x^2 \leqslant 2\sigma$. We shall find σ and β_1 such that $\langle \chi_{\sigma,x} \rangle_{\beta,h,\Lambda}^{\mathrm{cl}} \leqslant 1/2$, whence (ii) follows. By the chessboard estimate,[10]

$$\langle \chi_{\sigma,x} \rangle_{\beta,h,\Lambda}^{\mathrm{cl}} \leqslant \left[\left\langle \prod_{y \in \Lambda} \chi_{\sigma,y} \right\rangle_{\beta,h,\Lambda}^{\mathrm{cl}} \right]^{N^{-d}} \tag{14}$$

If $2\sigma < 1 - (h/h_0)^2$, the minimum energy on configurations satisfying $\rho_y^2 \leqslant 2\sigma$ for all y is again attained on parallel spins with maximum $\rho_y^2 = 2\sigma$, i.e., $H_{\Lambda}^{\mathrm{cl}} \geqslant -[2d\sigma + |h|(1-4\sigma^2)^{1/2}]\, N^d$. So, for some $E_1 < E_0$ one has, by choosing the appropriate σ, $H_{\Lambda}^{\mathrm{cl}} \geqslant -E_1 N^d$ on the interesting configurations. On the other hand, with $E_1 < E_2 < E_0$, one can find a neighborhood $V \subset \mathbf{S}^2$ of $(\rho^*, 0, (1-\rho^{*2})^{1/2})$ such that, if $s_y \in V$ for all $y \in \Lambda$, $H_{\Lambda}^{\mathrm{cl}}(\mathbf{s}) \leqslant -E_2 N^d$. Then

$$\left[\left\langle \prod_{y \in \Lambda} \chi_{\sigma,y} \right\rangle_{\beta,h,\Lambda}^{\mathrm{cl}} \right]^{N^{-d}} \leqslant \frac{e^{\beta E_1} \nu(\{\rho \leqslant 2\sigma\})}{e^{\beta E_2} \nu(V)} \tag{15}$$

which is less than 1/2 for β larger than some β_1.

In conclusion, the classical model has ferromagnetic long-range order at low temperature whenever the field is less than the value at which there is only one ground state with all spins pointing along the field.

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