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A rigorous theorem on off-diagonal long-range order of boson systems

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Abstract. For a strongly interacting boson system, it has been proposed that the concept of off-diagonal long-range ordering (ODLRO) is equivalent to Bose–Einstein condensation for a free boson system. Therefore, the existence of ODLRO in the ground state implies superfluidity. In this article, we check the validity of this proposition from another point of view. We shall rigorously show that, for a hard-core lattice-boson system with a short-ranged interaction, ODLRO is suppressed when a charged excitation gap develops and, hence, the boson system becomes a Mott-insulator. Finally, by using our theorem, we show some interesting properties of the antiferromagnetic Heisenberg model, which can be taken as a hard-core lattice-boson system.

It is well known that, in three-dimensions, a system of free boson particles undergoes a Bose–Einstein condensation and its ground state is superfluid. This phenomenon has been shown in the momentum representation. However, to a strongly interacting boson system, this representation may not be suitable any more. The strong correlation caused by interaction of particles renders the plane-wave picture poor to describe such a system. To remedy this problem, many new concepts and approximate methods have been proposed. Some of them can be found in a standard textbook [1]. In particular, in a remarkable article [2], Yang developed a theory of Penrose and Onsager [3, 4] and proposed off-diagonal long-range order (ODLRO). In contrast to the usual diagonal long-range order (DLRO), which represents a solid type ordering, Yang argued that the existence of ODLRO in the ground state of a strongly interacting boson system indicates superfluidity. Indeed, many boson systems, which are superfluids, do have ODLRO. For instance, numerical calculation shows that the ground state of ^4He supports ODLRO [1].

Naturally, one would not expect that all the strongly interacting boson systems have a superfluid ground state. In particular, if the interaction of particles causes a finite charged-excitation gap, the system will be a Mott-insulator, let alone a superfluid. In a very recent paper [5], Lee and Shanker showed that, for a two-dimensional hard-core lattice-boson system with a short-range interaction, a non-vanishing charged-excitation gap implies the existence of charge density wave commensurating with the lattice, i.e. diagonal long-range ordering, in the ground state. In other words, the boson system looks like a 'solid'. This picture is consistent with the definition of a Mott-insulator since the 'charged lattice' can be easily pinned down by an impurity and the system becomes insulating. Certainly, the ground state of this system must not be superfluid. Then, by Yang's argument, one would expect that ODLRO in the ground state is suppressed. Therefore, a charged-excitation gap and ODLRO cannot coexist. In

this article, for hard-core lattice-boson models, we give a direct and rigorous proof to the above conclusion and, hence, confirm Yang's argument. Then, by using our theorem, we show some interesting properties of the antiferromagnetic Heisenberg model, which can be taken as a hard-core lattice-boson system.

We first introduce some useful notation and terminologies.

Take a finite d -dimensional lattice Λ with N_Λ sites. For definiteness, we consider a simple cubic lattice. A hard-core lattice-boson system is defined by a Hamiltonian

$$H = tP \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j^\dagger b_i)P + V(b^+b) \quad (1)$$

where $t > 0$ is a parameter and P is a projection operator which annihilates the multiple-occupation configurations. $\langle ij \rangle$ denotes a pair of nearest-neighbour sites. b^+ (b) is the boson creation (annihilation) operator and $V(b^+b)$ represents a short-range interaction. We would like to emphasize that the sign of t does not matter very much. With respect to the Hamiltonian (1), a simple cubic lattice is bipartite. A proper canonical transformation can change the sign of t .

It is well known [5] that the Hamiltonian (1) is equivalent to a localized spin- $\frac{1}{2}$ Hamiltonian

$$H = t \sum_{\langle ij \rangle} (S_{i+}S_{j-} + S_{j+}S_{i-}) + V(S_z) \quad (2)$$

where $S_+ = S_x + iS_y$ and S_- is its Hermitian conjugate. Notice that the projection operator P is dropped in (2). Now, an occupied (unoccupied) site is represented by an up-spin (down-spin) and the number operator b^+b is replaced by $(1 + \sigma_z)/2$. For such a Hamiltonian, the total number of particles, N (equivalently, the number up-spins, N_\uparrow) is a conserved quantity. Let $E_0(N)$ be the energy of the ground state of this Hamiltonian in the sector of

$$N_\Lambda \geq N = N_\uparrow = \left\langle \Psi \left| \sum_{j \in \Lambda} \frac{1}{2}(1 + \sigma_{jz}) \right| \Psi \right\rangle. \quad (3)$$

A charged-excitation gap appears at filling $n_0 = N_0/N_\Lambda$ if there is a constant $e > 0$, which is independent of N_Λ , such that

$$\{E(N_0 + 1) - E(N_0)\} - \{E(N_0) - E(N_0 - 1)\} \geq e > 0. \quad (4)$$

In this case, adding a particle to the system costs more energy than removing one. Therefore, the system is insulating.

Next, let us recall the definition of ODLRO. Following Yang [2], for a ground state Ψ_0 of the Hamiltonian, its reduced two-particle matrix ρ_2 is defined by

$$(\rho_2)_{k,j} = \langle \Psi_0 | (Pb_k^+ P)(Pb_j P) | \Psi_0 \rangle = \langle \Psi_0 | S_{k+} S_{j-} | \Psi_0 \rangle \quad (5)$$

where k and j are two sites of Λ . By this definition, it is easy to see that ρ_2 is an $N_\Lambda \times N_\Lambda$ semipositive definite matrix. Let λ_1 be its largest eigenvalue. If there is a positive constant $c > 0$ independent of N_Λ satisfying

$$\lambda_1 \geq cN_\Lambda \quad (6)$$

then one can show that

$$\lim_{|k-j| \rightarrow \infty} (\rho_2)_{k,j} \neq 0 \quad (7)$$

i.e. Ψ_0 has ODLRO. On the other hand, it has been shown [6] that, when there is no external field, all the eigenvalues of ρ_2 have the following form

$$\lambda_q = \frac{1}{N_\Lambda} \sum_{k \in \Lambda} \sum_{j \in \Lambda} \langle \Psi_0 | S_{k+} S_{j-} | \Psi_0 \rangle \exp[iq \cdot (k - j)] \tag{8}$$

where q is a reciprocal vector of Λ . By introducing

$$S_{q-} = \frac{1}{\sqrt{N_\Lambda}} \sum_{j \in \Lambda} S_{j-} \exp(-iq \cdot j) \quad S_{q+} \equiv S_{q-}^\dagger \tag{9}$$

we can write λ_q in a simpler form

$$\lambda_q = \langle \Psi_0 | S_{q+} S_{q-} | \Psi_0 \rangle. \tag{10}$$

Therefore, Ψ_0 has ODLRO if and only if there is a reciprocal vector q_0 satisfying

$$\lambda_{q_0} = \langle \Psi_0 | S_{q_0+} S_{q_0-} | \Psi_0 \rangle \geq c N_\Lambda. \tag{11}$$

It is not difficult to see that ODLRO is the most natural extension of the concept of Bose-Einstein condensation to a strongly interacting boson system. Without interaction, S_{q+} is simply replaced by

$$b_q^+ \equiv \frac{1}{\sqrt{N_\Lambda}} \sum_{j \in \Lambda} b_j^+ \exp(-iq \cdot j). \tag{12}$$

The equation for Bose-Einstein condensation in the ground state Ψ_0

$$\lambda_0 = \langle \Psi_0 | b_{q=0}^+ b_{q=0} | \Psi_0 \rangle = N = n N_\Lambda \tag{13}$$

simply tells us that $\lambda_{q=0}$ is the largest eigenvalue of ρ_2 and it is a quantity of $O(N)$.

With these definitions, we now state our theorem in a precise form.

Theorem. Suppose that a hard-core lattice-boson system has a charged-excitation gap at filling $n_0 = N_0 / N_\Lambda$. Then, for any reciprocal vector q , λ_q can be, at most, $O(1)$ in the thermodynamic limit. Therefore, ODLRO is suppressed at n_0 .

Proof. Our proof is based on the following identity.

$$\langle \Psi_0 | [B^\dagger, [H, B]] | \Psi_0 \rangle = \sum_n (E_n - E_0) \{ |\langle \Psi_0 | B | \Psi_n \rangle|^2 + |\langle \Psi_0 | B^\dagger | \Psi_n \rangle|^2 \} \tag{14}$$

where B is an operator and B^\dagger is its Hermitian conjugate. $\{\Psi_n\}$ is a complete set of eigenvectors of the Hamiltonian H and $\{E_n\}$ are the corresponding eigenvalues. This identity can be easily checked by expanding the commutator and inserting the complete set $\{\Psi_n\}$ between operators.

We now let $B = S_{q-}$ and Ψ_0 be the ground state of H in the $N_\uparrow = N$. Notice that, only for Ψ_n in the sector of $N_\uparrow = N + 1$, the matrix element $\langle \Psi_0 | S_{q-} | \Psi_n \rangle$ is possibly non-zero. Similarly, if $\langle \Psi_0 | S_{q+} | \Psi_n \rangle$ is non-zero, then Ψ_n must be in the sector of $N_\uparrow = N - 1$. Therefore, identity (14) is now reduced to

$$\begin{aligned} \langle \Psi_0 | [S_{q+}, [H, S_{q-}]] | \Psi_0 \rangle &= \sum_n' (E_n(N-1) - E_0(N)) |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 \\ &\quad + \sum_m'' (E_m(N+1) - E_0(N)) |\langle \Psi_0 | S_{q-} | \Psi_m \rangle|^2. \end{aligned} \tag{15}$$

In (15), Σ' (Σ'') represents a partial sum over $N_\uparrow = N - 1$ ($N_\uparrow = N + 1$) sector. Since

$$E_n(N - 1) \geq E_0(N - 1) \quad \text{and} \quad E_n(N + 1) \geq E_0(N + 1) \quad (16)$$

the right-hand side of (15) is larger than

$$\begin{aligned} & \sum'_n [E_0(N - 1) - E_0(N)] \langle \Psi_0 | S_{q+} | \Psi_n \rangle^2 + \sum'_m [E_0(N + 1) - E_0(N)] \langle \Psi_0 | S_{q-} | \Psi_m \rangle^2 \\ &= \sum'_n \{ E_0(N + 1) - E_0(N) + E_0(N - 1) - E_0(N) \} \langle \Psi_0 | S_{q+} | \Psi_n \rangle^2 \\ & \quad + [E_0(N + 1) - E_0(N)] \left\{ \sum''_m |\langle \Psi_0 | S_{q-} | \Psi_m \rangle|^2 - \sum'_n |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 \right\} \\ & \geq e \sum'_n |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 + [E_0(N + 1) - E_0(N)] \\ & \quad \times \left\{ \sum''_m |\langle \Psi_0 | S_{q-} | \Psi_m \rangle|^2 - \sum'_n |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 \right\}. \end{aligned} \quad (17)$$

In the last step, we have used the definition of the charged-excitation gap. Obviously, each partial sum can now be replaced by the sum over the complete set $\{\Psi_n\}$. Therefore,

$$\begin{aligned} & \langle \Psi_0 | [S_{q+}, [H, S_{q-}]] | \Psi_0 \rangle \\ & \geq e \sum_n |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 + [E_0(N + 1) - E_0(N)] \\ & \quad \times \sum_n \{ |\langle \Psi_0 | S_{q-} | \Psi_n \rangle|^2 - |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 \} \\ & = e \sum_n |\langle \Psi_0 | S_{q+} | \Psi_n \rangle|^2 + [E_0(N + 1) - E_0(N)] \langle \Psi_0 | [S_{q-}, S_{q+}] | \Psi_0 \rangle. \end{aligned} \quad (18)$$

Since

$$[S_{q-}, S_{q+}] = -\frac{2}{N_\Lambda} \sum_{k \in \Lambda} S_{kz} \quad (19)$$

we have

$$\begin{aligned} & \langle \Psi_0 | [S_{q-}, S_{q+}] | \Psi_0 \rangle \\ & = -\frac{2}{N_\Lambda} \frac{1}{2} (N_\uparrow - N_\downarrow) = -\frac{1}{N_\Lambda} (2N_\uparrow - N_\Lambda) = 1 - 2\frac{N}{N_\Lambda} = 1 - 2n_0. \end{aligned} \quad (20)$$

Notice that the difference $E_0(N + 1) - E_0(N)$ is a quantity of $O(1)$ in the thermodynamic limit. Therefore, the second term on the right-hand side of (18) can be, at most, of $O(1)$.

Next, we estimate the averaged commutator $\langle \Psi_0 | [S_{q+}, [H, S_{q-}]] | \Psi_0 \rangle$.

We rewrite the Hamiltonian as

$$H = \left\{ t \sum_{\langle ij \rangle} (S_{i+} S_{j-} + S_{j+} S_{i-}) \right\} + V(S_z) = T + V. \quad (21)$$

For T , a direct calculation yields

$$\begin{aligned} & \langle \Psi_0 | [S_{q+}, [T, S_{q-}]] | \Psi_0 \rangle \\ & = \frac{2}{N_\Lambda} \langle \Psi_0 | -T | \Psi_0 \rangle + \frac{4t}{N_\Lambda} \left(\frac{1}{d} \sum_{m=1}^d \cos q_m \right) \left\langle \Psi_0 \left| -\sum_{\langle ij \rangle} S_{iz} S_{jz} \right| \Psi_0 \right\rangle \end{aligned} \quad (22)$$

where q_m is the component of q in the e_m direction and d is the dimension of the lattice. Since T and

$$L = \sum_{\langle ij \rangle} S_{iz} S_{jz} \tag{23}$$

are sums of nearest-neighbour-paired operators, one would expect that the following inequalities hold

$$0 \leq \langle \Psi_0 | -T | \Psi_0 \rangle \leq \alpha z t N_\Lambda \quad 0 \leq \langle \Psi_0 | -L | \Psi_0 \rangle \leq \beta N_\Lambda \tag{24}$$

where α and β are positive constants independent of N_Λ and $z = 2d$ is the number of the nearest-neighbours of each lattice site. These upper bounds can be rigorously shown by using Gershgorin's theorem. First, we define an order among the lattice sites by alphabetical order and then introduce a basis, which spans the Hilbert subspace without multiple occupation by

$$\Phi_\alpha \equiv S_{j_1+} S_{j_2+} \dots S_{j_N+} |F\rangle. \tag{25}$$

In this definition, $|F\rangle$ denotes the spin configuration with all the spins downwards. α is a choice of (j_1, j_2, \dots, j_N) , which are the positions of the N up-spins. In terms of this basis, we write T and L in matrices. The matrix L is diagonal. Therefore, its non-zero elements are its eigenvalues. A little calculation yields the second inequality of (24). For T , we observe that all of its diagonal elements are zero and its non-vanishing elements are $-ts$. Furthermore, in each row of matrix T , there are at most zN non-zero elements. Therefore, the upper bound for $-T$ is a direct corollary of the following lemma due to Gershgorin.

Lemma (Gershgorin's theorem). Let A be an $M \times M$ matrix. Then, any eigenvalue λ of A satisfies the following inequality

$$|\lambda| \leq \max_i \sum_{j=1}^M |a_{ij}|. \tag{26}$$

One can find a proof of Gershgorin's theorem and its application to Nagaoka theorem in [7] and [8].

Substituting (24) into (23), we find that

$$\langle \Psi_0 | [S_{q+}, [-T, S_{q-}]] | \Psi_0 \rangle = O(1) \tag{27}$$

for any q .

For $V(S_z)$, if it is short ranged with a finite maximum interaction intensity, V_{\max} , then the above argument also applies. Since $V(S_z)$ is a sum of products of (S_{iz}) , $\langle \Psi_0 | [S_{q+}, [V(S_z), S_{q-}]] | \Psi_0 \rangle$ does not contain any singular term. Assume that the effective range of $V(S_z)$ is R_0 . By Gershgorin's theorem, we can easily show that

$$|\langle \Psi_0 | [S_{q+}, [V(S_z), S_{q-}]] | \Psi_0 \rangle| \leq \gamma R_0^d V_{\max} = O(1) \tag{28}$$

where γ is a positive constant independent of N_Λ . In summary,

$$\begin{aligned} &\langle \Psi_0 | [S_{q+}, [H, S_{q-}]] | \Psi_0 \rangle \\ &= \langle \Psi_0 | [S_{q+}, [T, S_{q-}]] | \Psi_0 \rangle + \langle \Psi_0 | [S_{q+}, [V(S_z), S_{q-}]] | \Psi_0 \rangle \\ &= O(1). \end{aligned} \tag{29}$$

Combining (18), (20) and (29), we finally obtain

$$O(1) \geq e \langle \Psi_0 | S_{q+} S_{q-} | \Psi_0 \rangle. \tag{30}$$

It holds for any reciprocal momentum q . If the charged-excitation gap e does not vanish, then $\lambda_q = \langle \Psi_0 | S_{q+} S_{q-} | \Psi_0 \rangle$ can be, at most, $O(1)$ for arbitrary q . Therefore, by definition, Ψ_0 does not support ODLRO.

Our proof is accomplished. □

As an application of our theorem, let us consider the following Hamiltonian

$$H = t \sum_{\langle ij \rangle} (S_{i+} S_{j-} + S_{j+} S_{i-}) + U \sum_{\langle ij \rangle} S_{iz} S_{jz} \tag{31}$$

where $U > 0$ is a parameter. In particular, when $t = 2U$, the Hamiltonian is the wellknown spin- $\frac{1}{2}$ antiferromagnetic Heisenberg model. It has been shown [9–11] that, in three dimensions, the non-degenerate ground state of the Heisenberg model has the total spin number $S = 0$ and supports an antiferromagnetic long-range order. Using the notation of [11], this ordering can be explicitly expressed as

$$g_Q = \langle \Psi_0 | S_{Qz}^+ S_{Qz} | \Psi_0 \rangle \geq \delta N_\Lambda \tag{32}$$

where $Q = (\pi, \pi, \pi)$ and $\delta > 0$ is a constant independent of N_Λ . In other words, the hard-core lattice-boson system represented by the Heisenberg Hamiltonian has DLRO at filling $n_0 = \frac{1}{2}$. In the following, we shall show that it also has ODLRO at the same filling. Then, by our theorem, the system has a vanishing charged-excitation gap and, hence, cannot be an insulator. On the other hand, when $U \gg t$, the Hamiltonian reduces to an Ising model, whose ground state is the Neel state and has a charged-excitation gap $e \sim 2U$. Therefore, DLRO still exists but ODLRO is suppressed. The system is insulating. In summary, we find that there exist $U_{c1} < U_{c2}$ such that, when $U < U_{c1}$, the system is superfluid and when $U > U_{c2}$, it is insulating. So far, we cannot determine whether $U_{c1} = U_{c2}$.

Now, we show that the Heisenberg Hamiltonian has ODLRO at filling $n_0 = \frac{1}{2}$. First, we notice that, for a pair of lattice points k and j ,

$$\langle \Psi_0 | S_{kx} S_{jx} | \Psi_0 \rangle = \langle \Psi_0 | S_{ky} S_{jy} | \Psi_0 \rangle = \langle \Psi_0 | S_{kz} S_{jz} | \Psi_0 \rangle. \tag{33}$$

Intuitively, that is due to the fact that the Heisenberg Hamiltonian is isotropic in spin space and, hence, one cannot single out a special direction. Formally, this identity can be rigorously proven by noticing that the Hamiltonian commutes with the following spin operators:

$$S_\xi \equiv \sum_{j \in \Lambda} S_{j\xi} \quad \xi = x, y, z. \tag{34}$$

Therefore, H is invariant under the unitary transformations

$$U_\xi \equiv \exp \left\{ i \frac{\pi}{2} S_\xi \right\} \tag{35}$$

and any subspace spanned by the eigenvectors of H with the same eigenvalue E is also invariant under U_ξ . In particular, since the ground state Ψ_0 in $S = 0$ sector is non-degenerate, it must satisfy

$$U_\xi | \Psi_0 \rangle = \exp \left\{ i \frac{\pi}{2} S_\xi \right\} | \Psi_0 \rangle = \exp \{ i \alpha_\xi \} | \Psi_0 \rangle \tag{36}$$

where α_ξ is a constant dependent of ξ . Let $\xi = y$. Then,

$$\begin{aligned} \langle \Psi_0 | S_{kx} S_{jx} | \Psi_0 \rangle &= \langle \Psi_0 | (U_y^\dagger U_y) S_{kx} (U_y^\dagger U_y) S_{jx} (U_y^\dagger U_y) | \Psi_0 \rangle \\ &= \langle \Psi_0 | \exp(-i\alpha_y) (U_y S_{kx} U_y^\dagger) (U_y S_{jx} U_y^\dagger) \exp(i\alpha_y) | \Psi_0 \rangle \\ &= \langle \Psi_0 | S_{kx} S_{jx} | \Psi_0 \rangle. \end{aligned} \tag{37}$$

Similarly, by letting $\xi = x$, we obtain the second part of identity (33).

Another observation which we need is that, for two distinct points k and j ,

$$\langle \Psi_0 | S_{kx} S_{jy} | \Psi_0 \rangle = 0. \tag{38}$$

It is due to the following simple facts.

(i) The operator $S_{kx} S_{jy}$ is Hermitian when k and j are distinct. Therefore, its expectation in Ψ_0 is a real quantity.

(ii) As the unique ground state of H , which is a real Hamiltonian, Ψ_0 is a real linear combination of basis vectors. But, $S_{kx} S_{jy}$ is an imaginary operator. Therefore, its expectation in Ψ_0 must be an imaginary quantity.

Combining (i) and (ii), we see that (38) holds.

With equations (33) and (38), we find

$$\begin{aligned} \langle \Psi_0 | S_{q+} S_{q-} | \Psi_0 \rangle &= \frac{1}{N_\Lambda} \sum_{k \in \Lambda} \sum_{j \in \Lambda} \exp(i\mathbf{q} \cdot (\mathbf{k} - \mathbf{j})) \langle \Psi_0 | S_{k+} S_{j-} | \Psi_0 \rangle \\ &= \frac{1}{N_\Lambda} \sum_{k \in \Lambda} \sum_{j \in \Lambda} \exp(i\mathbf{q} \cdot (\mathbf{k} - \mathbf{j})) \\ &\quad \times \langle \Psi_0 | S_{kx} S_{jx} + S_{ky} S_{jy} + i S_{ky} S_{jx} - i S_{kx} S_{jy} | \Psi_0 \rangle \\ &= \frac{1}{N_\Lambda} \sum_{k \in \Lambda} \sum_{j \in \Lambda} \exp(i\mathbf{q} \cdot (\mathbf{k} - \mathbf{j})) \langle \Psi_0 | 2 S_{kz} S_{jz} | \Psi_0 \rangle \\ &\quad + \frac{1}{N_\Lambda} \left\langle \Psi_0 \left| \sum_{k \in \Lambda} S_{kz} \right| \Psi_0 \right\rangle \\ &= 2 \langle \Psi_0 | S_{qz}^+ S_{qz} | \Psi_0 \rangle. \end{aligned} \tag{39}$$

In the last step, we have used the fact that Ψ_0 has quantum number $S_z = 0$. Equation (39) holds for any \mathbf{q} . In particular, it holds for $\mathbf{q} = \mathbf{Q}$. Therefore,

$$\langle \Psi_0 | S_{Q+} S_{Q-} | \Psi_0 \rangle = 2 \langle \Psi_0 | S_{Qz}^+ S_{Qz} | \Psi_0 \rangle \geq 2\delta N_\Lambda \tag{40}$$

i.e. there is also ODLRO in Ψ_0 .

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