Bi-partite mode entanglement of bosonic condensates on tunnelling graphs

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We study a set of $L$ spatial bosonic modes localized on a graph $\Gamma$. The particles are allowed to tunnel from vertex to vertex by hopping along the edges of $\Gamma$. We analyze how, in the exact many-body eigenstates of the system i.e., Bose-Einstein condensates over single-particle eigenfunctions, the bi-partite quantum entanglement of a graph vertex with respect to the rest of the graph depends on the topology of $\Gamma$.

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The possibility of exploiting the quantum features of bosonic particles e.g., cold bosonic atoms, living on coupled spatial lattices to the aim of Quantum Information Processing (QIP) [1] has been recently addressed in the literature [2, 3, 4, 5]. These systems provide also a unique opportunity to investigate fascinating coherent phenomena e.g., quantum-phase transitions [6].

In this note we shall study a simple problem related to this more general context. We shall consider a set of $N$ bosonic particles hopping between the $L$ vertices of a graph $\Gamma$, we will assume the on-vertex self-interaction terms to be zero. The associated elementary quadratic Hamiltonian is exactly solvable and many-body eigenstates are simply given by Bose-Einstein condensates (BECs) over single-particle wavefunctions. This kind of abstract situation could be realized, for instance, in a optical lattice loaded with cold atomic atoms that can tunnel from different local traps and with atom self-interactions somehow switched off [7].

The aim is to analyze the role of the graph topology in determining, in those many-body eigenstates, the bi-partite quantum entanglement of a vertex with respect to the rest of the graph vertices. In particular one can address the issue of bi-partite entanglement in the ground-state of the system and how e.g., for QIP purposes to optimize it by graph designing (for a related study see [7, 8, 9]).

It is worthwhile to stress that in this paper the view of quantum entanglement in system of indistinguishable particles is the one based on modes advocated in Refs. [10, 11, 12] rather than the complementary one based on particles [13].

Let us start by recalling the basic kinematical framework an to lay down the basic notations. The quantum state-space associated with graph $\Gamma$ is given by the tensor product of $L$ linear oscillator Fock spaces $H_{\Gamma} \equiv \otimes_{j \in \Gamma} \text{span}\{|n_j\rangle\}_{n_j=0}$. Since we are mostly interested in massive particles e.g., atoms, we will focus on sectors of $H_{\Gamma}$ with definite total particles number

$$H_{\Gamma}^{(N)} := \text{span}\{\otimes_{j=1}^L |n_j\rangle / \sum_{j=1}^L n_j = N \}. \quad (1)$$

Given a state $|\Psi\rangle \in H_{\Gamma}^{(N)}$ we are here interested to the on-site reduced density matrix; if $|\Psi\rangle = \sum_{n_1, \ldots, n_L} C(n_1, \ldots, n_L) \otimes_{j=1}^L |n_j\rangle$ one has, say for the first vertex

$$\rho^{(1)} := \text{Tr}_{\Gamma-\{1\}}|\Psi\rangle\langle\Psi| = \sum_{m=0}^N \rho_{m}^{(1)}|m\rangle\langle m|,$$

where $1)$ the $b_i$’s are bosonic modes, 2) $A := (A_2^{0})_{ij} \in M_L(Z_2)$, $(Z_2 = \{0, 1\})$ is an symmetric matrix. We will consider the case in which $A$ is an adjacency matrix of a graph $\Gamma = (V, E)$, where $V = \{1, \ldots, L\}$ is the set of vertices and $E$ is the set of edges, $(i, j) \in E$ iff $A_{ij} \neq 0$.

By diagonalizing $A$ one gets $H[A] = \sum_{k=1}^L \omega_k B_k^\dagger B_k$, where $\omega_k$ are the $A$-eigenvalues and $B_k^\dagger B_k$ are new bosonic modes ($U \in M_L(\mathbb{C})$ is unitary).

Let us now consider a non-degenerate eigenvalue $\omega_1$ of $A$ and a $N$ particles condensate over it. If $B_1 = (U_{11}, U_{12}, \ldots, U_{1L})$ denotes the associated eigenvector, one has

$$|B_1^N\rangle := \frac{1}{\sqrt{N!}} (B_1^0) |0\rangle = \frac{1}{\sqrt{N!}} \sum_{i_1, \ldots, i_N} \prod_{k=1}^N U_{1,k} b_k^\dagger |0\rangle$$

$$= \sqrt{\frac{N!}{\prod_{k=1}^N n_k!}} \otimes_{k=1}^L U_{1,k}^n |n_k\rangle \quad (4)$$

The reduced density matrix associated to the ith mode is given by

$$\rho^{(i)} := \text{Tr}_{\Gamma-\{i\}}|B_1^N\rangle\langle B_1^N| = \sum_{m=0}^N \rho_{m}^{(i)}(B_1)|m\rangle\langle m| \quad (5)$$

where

$$\rho_{m}^{(i)}(B_1) = \sum_{\{j_n\} \in S_N(i,m)} \prod_{n=1}^N |U_{1,j_n}|^2$$

The prime in the above sum simply reminds that the condition $\sum_{j=2}^L = N - m$ must be fulfilled. The crucial, though obvious thing, to notice here is that the constraint of fixed total particle-number results in a diagonal reduced density matrix, and that such a matrix can be always seen as an operator over the finite-dimesional space $\mathbb{C}^M$ with $M \geq N$. This remark relieves us to face with the subtleties of entanglement definition in truly infinite-dimensional spaces [14].

Let the hamiltonian be

$$H[A] = -\sum_{i,j=1}^L A_{ij} b_i^\dagger b_j \quad (3)$$

and many-body eigenstates are simply given by Bose-Einstein condensates (BECs) over single-particle eigenfunctions. This kind of abstract situation could be realized, for instance, in a optical lattice loaded with cold atomic atoms that can tunnel from different local traps and with atom self-interactions somehow switched off [7].

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$$\rho^{(1)} := \text{Tr}_{\Gamma-\{1\}}|\Psi\rangle\langle\Psi| = \sum_{m=0}^N \rho_{m}^{(1)}|m\rangle\langle m|,$$
function i.e., non necessarily an Eq. (9) defines – for any given vertex that the Neumann entropy of the reduced density matrix is given by \( S(\rho^{(i)}(B_1)) = -\text{Tr}(\rho^{(i)} \log_2 \rho^{(i)}) \)

\[
\rho^{(i)}_m(B_1) = \binom{N}{m} |U_{1,i}|^{2m} (1 - |U_{1,i}|^2)^{N-m}
\]

This expression is the result we needed. Clearly Eq. (8) has a very simple meaning: the probability \( p \) of occupying the vertex \( i \) (\( \Gamma - \{i\} \)) in the single-particle wavefunction \( B_1 \) is given by \( |U_{1,i}|^2 \). Since the BEC over \( B_1 \) is the tensor-product of \( N \) copies of \( B_1 \) the probability \( \rho^{(i)}_m \) of having \( m \)-particle on \( i \) is given by a binomial distribution \( \binom{N}{m} p^m (1-p)^{N-m} \). This classical argument works because of the fixed particle-number constraint forces the vertex reduced density matrix to be diagonal i.e., a probability distribution.

From now on we will measure entanglement by the von Neumann entropy of the reduced density matrix

\[
e_N^{(i)}(B_1) := S(\rho^{(i)}(B_1)) = -\text{Tr}(\rho^{(i)} \log_2 \rho^{(i)}) = -\sum_{m=0}^{N} \rho^{(i)}_m \log_2 \rho^{(i)}_m
\]

By noting that \( B_1 \) can be an arbitrary single-particle wavefunction i.e., non necessarily an \( H[A] \) eigenstate, one realizes that Eq. (6) defines – for any given vertex \( i \) of \( \Gamma \) – a positive real-valued function over the single-particle space i.e., \( e_N^{(i)} : \mathbb{M}^L \rightarrow \mathbb{R}_+ \). From expression (8) one readily show that

- The entanglement of a vertex with respect to the others in a BEC depends only on the square amplitude, over the considered site, of the single-particle eigenstate we are condensing over.

More formally \( e_N^{(i)}(W x) = e_N^{(i)}(x) \), (\( \forall x \in \mathbb{M}^L \)) for unitaries \( W \) belonging to the group \( U(1) \times U(L-1) \) (phase on the \( i \)-th component, arbitrary unitary mixing of the all the other ones). This invariance is, of course, nothing but the invariance of entanglement with respect to local transformations.

- The graph size \( L \) does not enter in entanglement properties, but possibly through the single particle amplitude \( |U_{1,i}| \).

- It is easy to prove that the functions \( e_N^{(i)} \)'s have a maximum for \( U_{1,i} = 1/\sqrt{2} \) (see Fig. 3).

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\[
= \sum_{\{n_k\} \in \mathcal{S}_N(i,m)} N^L \prod_{l=1}^{L} \frac{1}{|q_l|} |U_{1,l}|^{2n_l},
\]

where

\[
\mathcal{S}_N(i,m) = \{(j_n) \in \mathbb{N}^N_L / \#\{j_n = i\} = m\}
\]

\[
\mathcal{S}_N(i,m) := \{(n_l) \in \mathbb{N}^L_N / \sum_{l=1}^{L} n_l = N, n_i = m\}. (7)
\]

Now, using the fact that \( \sum_{j=1}^{L} |U_{1,j}|^2 = 1 \) is not difficult to see that one can further rearrange the last expression in Eq. (6) in order to get

\[
\rho^{(i)}_m(B_1) = \binom{N}{m} |U_{1,i}|^{2m} (1 - |U_{1,i}|^2)^{N-m}
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By noting that \( B_1 \) can be an arbitrary single-particle wavefunction i.e., non necessarily an \( H[A] \) eigenstate, one realizes that Eq. (6) defines – for any given vertex \( i \) of \( \Gamma \) – a positive real-valued function over the single-particle space i.e., \( e_N^{(i)} : \mathbb{M}^L \rightarrow \mathbb{R}_+ \). From expression (8) one readily show that

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\[
\Gamma \in \mathcal{G}_L, \rightarrow \max_{k} e_N^{(i)}(B_k(\Gamma))
\]

One could restrict the problem, by considering just the eigenvector \( B_1(\Gamma) \) associated with the largest eigenvalue of the adjacency matrix of \( \Gamma \). This eigenvector corresponds then (see Eq. (9)) to the lowest single-particle energy and the BEC \( |B_1^\Gamma\rangle \) is a many-body ground state of the Hamiltonian \( \hat{H} \). By the Perron-Frobenius theorem \( \hat{H} \) we know that –for connected \( \Gamma - B_1 \) is elementwise positive and that the associated eigenvalue is nondegenerate, hence the ground state is unique.
To exemplify this problem let us consider as $\Gamma$ the complete graph minus the diagonal i.e., $A[\Gamma] = \sum_{i,j=1}^{L}(1-\delta_{ij})|i\rangle\langle j|$. By writing this matrix in the following form $A[\Gamma] = L[X](X-I)$, $|X| := L^{-1/2}\sum_{j=1}^{L}|j\rangle$, one immediately realizes that the $A$ spectrum is given by $L - 1$ (with eigenvector $|X\rangle$) and by 0 with associated the the $L - 1$ operators $b_k$, $(k = 1, \ldots, L - 1)$. The $N$-particle ground state is therefore provided by putting the $N$ in the $k = 0$ bosonic mode associated with $X$. The ground-state bi-partite entanglement is given by $\|\Psi\rangle$ and $\|\tilde{\Psi}\rangle$ with $|U_{i,j}| = L^{-1/2}$.

If $\Gamma$ is a regular graph with connectivity $r$ i.e., all the vertices have $r$ neighbors, it is fact of elementary spectral graph theory [15] that the highest eigenvalue of the $\Gamma$ adjacency matrix is given by $r$ and the associated eigenvector is given by the 0 Fourier mode $1/\sqrt{L}(1, \ldots, 1)$. Therefore for regular graphs maximal bi-partite entanglement is possible just for the dimer i.e., $L = 2$. Notice that for the more general case of one-dimensional rings with $L$ (diagonalized by Fourier transformation with cyclic boundary conditions) the same value of (9) is achieved for all the vertices in all the BECs in single particle states. This fact stems from translational invariance which implies that all the single-particle eigenfunctions have the same vertex square amplitude i.e., $L^{-1}$.

It is interesting to note in passing that the bi-partite graphs ($V = A \cup B$, $(a, b) \in E \Leftrightarrow a \in A$ and $b \in B$) the mode entanglement associated with BEC over the single-particle eigenvalue $E$ is the same as the one with eigenvalue $-E$. One can realize this fact by performing the following canonical transformation in the Fock space associated with the $\Gamma$ modes: $c_j \rightarrow (-1)^{\chi_A(j)}c_j$, where $\chi_A$ denotes the characteristic function of the sub-graph $A$. One has that $H[A] \rightarrow H[-A] = -H[A]$, and that the $H[A]$ eigenvectors change their components over the Fock basis $\otimes_{j=1}^{N}|n_j\rangle_j$ just by a phase factor $\exp(i\pi \sum_{j \in A} n_j)$. Then the claim follows straight away from Eq. (9). Notice also that this symmetry property implies that for any initial state $|\Psi\rangle$ (not necessarily an $H[A]$ eigenstate) the on-vertex entanglement dynamics is invariant under time-reversal, i.e., $S(t) = S(-t)$, and moreover this result holds even in presence of local Hubbard-like self interactions [14].

For a general number of vertices $L$, the natural question is:

What is the graph topology which optimize the on-vertex entanglement?

The answer is not difficult to find out. Let $A$ be the adjacency matrix of the “star” i.e., just the node $1$ is connected to all the others, $A_{i,j} = \delta_{i,1}$. This matrix has two non zero eigenvalues $e_{\pm} = \pm\sqrt{L-1}$ corresponding to the single-particle operators

$$b_{\pm} := \frac{1}{\sqrt{2}}(b_1 \pm \frac{1}{\sqrt{L-1}}\sum_{j=1}^{L} b_j).$$

The $N$-particle ground state is unique and is given by $|b_N^{+}\rangle = (b_1)^N/\sqrt{N!}|0\rangle$. In view of Eqs. (9) and (12) the functional $e_N$ is maximized for all $N$ by the star graph. Physically this means that the star topology optimizes the bi-partite entanglement in the ground-state BEC. In view of the “monogamy” properties of quantum entanglement [9] this result looks, in a sense, rather intuitive. A naive argument is that the star topology is the one with maximall connectivity of the vertex 0 with the subgraph with $V = \{1, \ldots, L - 1\}$, this latter in turn is totally disconnected and therefore among its vertices there is small entanglement.

In this brief report we studied the mode entanglement in Bose-Einstein condensate over a purely tunnel-coupled graph. We found an exact expression for such a quantity for arbitrary graph and particle number. We proved that the star topology maximizes the bi-partite entanglement of the spatial mode associated to the star center with the rest of the vertices. The role of local self-interaction i.e., non-linear terms, as long as the practical relevance e.g., implementation, QIP protocols, of our abstract though simple analysis is subject of ongoing investigations [16].

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[1] D.P. DiVincenzo and C. Bennett, Nature 404, 247 (2000).
[2] D. Jaksch et al., Phys. Rev. Lett. 81, 3108 (1998).
[3] Z.B. Chen and Y.D. Zhang, Phys. Rev. A 65, 022318 (2002).
[4] R. Ionicioiu, P. Zanardi, Phys. Rev. A 66, 050301(R) (2002)
[5] L.M. Duan et al., quant-ph/0105056, Durner et al., quant-ph/0212039
[6] M. Greiner et al., Nature 415, 39 (2002).
[7] R. Burioni et al J. Phys. B 34 4697 (2001)
[8] C. Simon, Phys. Rev. A 66, 052323 (2002)
[9] A. P. Hines et al quant-ph/0209122
[10] P. Zanardi, Phys. Rev. A 65, 042101 (2002); P. Zanardi, X-G. Wang, J. Phys. A: Math. Gen., 35, 7947 (2002)
[11] J. R. Gittings and A. J. Fisher, Phys. Rev. A 66, 032305 (2002)
[12] Yu Shi, quant-ph/0205065, quant-ph/0204058, van Enk, quant-ph/0206135
[13] J. Schliemann, D. Loss, and A. H. MacDonald, Phys. Rev. B 63, 085311 (2001); J. Schliemann, J. I. Cirac, M. Kuś, M. Lewenstein, and D. Loss, Phys. Rev. A 64, 022303 (2001).
[14] J. Eisert, C. Simon, M. Plenio, J. Phys A 35, 3911 (2002); M. Keyl, D. Schlingemann, R. F. Werner, quant-ph/0212014
[15] Chris D. Godsil, Gordon F. Royle, Algebraic Graph Theory, Graduate Texts in Mathematics, Springer Verlag (2001)
[16] P. Giorda, P. Zanardi, in preparation