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No Bose-Einstein Condensation in Closed Systems with Linear Dynamics

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Abstract. Recently Bose-Einstein condensation has gathered a popularity and interest. An interesting theoretical phenomenon closely related to BEC and condensation is Frohlich's dynamic condensation phenomenon, proposed as a reoccurring mechanism in biophysics. This phenomenon studied classically brings forth a hypothesis that dynamic emergence of condensation requires nonlinear interactions. Working in the purely quantum regime I show the correctness of the hypothesis for a broad class of initial states as well as show a way for condensation to emerge from linear dynamics if the initial state has very large or very long-range quantum correlations.

Keywords: quantum thermodynamics, non-equilibrium, Bose-Einstein condensation

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1. Introduction

Bose-Einstein condensation (BEC) is a phase transition observed in quantum thermodynamic matter, where the occupation number in a single mode takes on a macroscopic value under some critical temperature. This phenomenon is paradigmatic for superconductivity and superfluidity, and has applications in quantum technologies, optical-lattice studies etc [1-5]. A significant application for BEC is the ability to make ultra-precise measurements. The high coherence of the BEC states can be used to drastically improve the precision of interferometry [6-8].

More than a half of century ago (i.e. much before the recent surge of interest related to BEC in atomic gases), Frohlich suggested that a phenomenon of BEC can be realized for non-linearly interacting, non-equilibrium phonons under influx of energy [9-11]. He was motivated by general features of order and coherence associated with BEC, and proposed that it can have direct applications in those biophysical situations, where a large-scale coherence is involved, e.g. conformational motion in biopolymers or impulse propagation in nerves.

Frolich's BEC is a dynamic phenomenon, where instead of lowering the temperature below its critical value (which is the standard scenario of equilibrium BEC), the system is dynamically brought to a state where a single mode has a macroscopic occupation number. This phenomenon has been derived using a classical model for the phonons and the bath, where it has been shown that the non-linearity of interactions between different modes is required for the emergence of the condensate. This phenomenon has also been derived in a quantum system with nonlinear interactions [12-14].

The ideas of Frohlich so far did not find direct applications in biophysics. Nevertheless, deep physical features of his approach invite further considerations that will certainly enrich our understanding of BEC itself. Starting from Frohlich's works, we revisit here the important topic of nonlinearity as a requirement for dynamical realization of BEC. Note that in the theory of BEC, the nonlinearity is commonly interpreted as the cubic term in the Gross–Pitaevskii equation [15]. Such a term comes from the mean-field approach, where the Schroedinger equation for a many-boson system is converted into a nonlinear equation for a single effective quasi-particle. Here, we understand the nonlinearity more fundamentally, as the non-quadratic terms in inter-mode interaction Hamiltonian. Our definition of nonlinearity can also exist for just two bosonic modes and provides an important resource for quantum thermodynamic tasks [16]. In particular, it has been shown (for a general class of initial states in boson systems) that a linear evolution in bosonic systems increases the mean number of excitations, a phenomenon that can be associated with the noise increase [17, 18]. Likewise, noise reduction is possible due to non-linear inter-mode interactions [18].

My main result here is that in a closed system for a large class of states, the phenomenon of BEC is dynamically impossible if all interactions are linear and initial conditions do not contain implanted inter-mode correlations. I relate the mechanism of this result to the maximal work-extraction problem. I also show that linear interactions can lead to condensation for an initial state that does not satisfy the mentioned condition. Thereby, I make Frohlich's classical hypothesis about the relevance of nonlinearity for BEC more precise in the quantum regime.

2. Setup and Dynamics

A closed many-mode boson system is described by the Hamiltonian ($\hbar = 1$)

$$H = \sum_{i=1}^{r} \omega_i a_i^\dagger a_i + H_I = H_0 + H_I, \qquad 1)$$

where r is the number of modes, ω_i is the frequency of the mode (in ascending order), a_i, a_i^+ are the annihilation and creation operators, and H_I is the interaction Hamiltonian. The commutation relations read

$$[a_i,\, a_i^\dagger] = \delta_{ij}, \qquad 2)$$

where δ_{ij} is the Kronecker delta. We take an interaction Hamiltonian depending on some external control parameter $\lambda(t)$ such that $H_I(t<0) = H_I(t>\tau) = 0$. We start from some general non-equilibrium initial state ρ (density matrix) that satisfies the following properties

$$\begin{aligned} tr(\rho a_j) &= \langle a_j \rangle = 0, \\ tr(\rho a_j a_k) &= \langle a_j a_k \rangle = 0, \\ tr(\rho a_j a_k^\dagger) &= \langle a_j a_k^\dagger \rangle = 0. \end{aligned} \qquad 3)$$

I consider (3) as a reasonable candidate for a quasi-stable (hydrodynamic type) non-equilibrium stationary state. Indeed, note that in the interaction representation with respect to (1) we get $a_k \propto e^{-i\omega_k t}$, i.e. the terms involved in (3) are rapidly oscillating except for the third equation when $\omega_k \approx \omega_j$.

2.1. Linear Heisenberg evolution

The interaction Hamiltonian H_I being quadratic in the creation and annihilation operators leads to a simple linear time evolution in the Heisenberg picture of said operators. For $a_j = a_j(0)$ and $b_j = a_j(\tau)$ operators it results in

$$b_i = \sum_{j=1}^{r} \left(S_{ij} a_j + R_{ij} a_j^\dagger \right) + f_i, \qquad 4)$$

where from the commutation relations

$$[b_i,\ b_i^\dagger] = \delta_{ij}, \tag{5}$$

we get

$$SS^\dagger - RR^\dagger = I, \qquad SR^T = RS^T,$$
$$S^\dagger S - R^T R^* = I, \qquad S^\dagger R = R^T S^*. \tag{6}$$

Thus the change in the occupation number of mode i equals

$$\begin{aligned} n_i(\tau) - n_i(0) &= \langle\, b_i^\dagger b_i\rangle - \langle\, a_i^\dagger a_i\rangle \\ &= |f_i|^2 + \sum_{j,k=1}^{r} \left[\, S_{ij}^* S_{ik} \langle\, a_j^\dagger a_k\rangle + \ R_{ij}^* R_{ik} \langle a_j\ a_k^\dagger\rangle\right] - \langle\, a_i^\dagger a_i\rangle. \end{aligned} \tag{7}$$

Following the derivations in [18] we arrive to the equation

$$\begin{aligned} \Delta n = \ \sum_{i=1}^{r} n_i(\tau) - n_i(0) &= \sum_{i=1}^{r} \langle\, b_i^\dagger b_i\rangle - \langle\, a_i^\dagger a_i\rangle \\ &= \sum_{i=1}^{r} \left(|f_i|^2 + \sum_{j=1}^{r} \left|R_{ij}\right|^2 \right) + 2 \sum_{i,j,k=1}^{r} R_{ij} R_{ik}^* \langle\, a_j^\dagger a_k\rangle \geq 0. \end{aligned} \tag{8}$$

Equations (6, 7, 8) show that the occupation number of a single mode can be increased in a linear process by any value desirable. This, however, is achieved by pumping a specific mode $|f_i|$ or by beneficially swapping a_i with $a_j^\dagger$ via R_{ij}, which results in an increase of the occupation numbers in several modes. A simple example of the latter can be obtained by the matrices S, R written in block matrix form as

$$\mathrm{S} = \begin{bmatrix} \hat{A} & 0 \\ 0 & \hat{I} \end{bmatrix}, \quad R = \begin{bmatrix} \hat{B} & 0 \\ 0 & 0 \end{bmatrix}, \tag{9}$$

where $\hat{I}$ is the $r-2$ dimensional identity matrix and

$$\hat{I} = \begin{bmatrix} \sqrt{N+1} & 0 \\ 0 & \sqrt{N+1} \end{bmatrix}, \quad R = \begin{bmatrix} 0 & \sqrt{N} \\ \sqrt{N} & 0 \end{bmatrix}, \tag{10}$$

This evolution achieves a change in the occupation number of the first two modes $\Delta n_{1,2} \ = \ N n_{1,2}$.

Evidently both of the discussed cases can infinitely pump energy into specific modes to raise their occupation numbers and this is not of particular interest to condensation. Below we will discuss the cases where the mean boson number of the closed system is kept constant. These states are of particular interest for molecular BEC [4, 5] and trapped boson systems [19].

3. Constant mean boson number

From (7) using (6) we find that the only type of linear dynamics that preserves the mean boson number is $f_i = R_{ij} = 0$ and unitary S, therefore,

$$n_i(\tau) = \sum_{j=1}^{r} M_{ij} n_j(0) \tag{11}$$

where $M_{ij} = \left|S_{ij}\right|^2$ is a double stochastic matrix. Now the change in energy and the change in the occupation number of some fixed mode are equal to

$$\begin{gathered} \Delta E = \sum_{i,j=1}^{r} \left(M_{ij} - \delta_{ij}\right) \omega_i n_j(0) \\ \Delta n_i = \sum_{j=1}^{r} M_{ij} n_j(0) - n_i(0) \end{gathered} \tag{12}$$

3.1. Maximum occupation in one mode

As Δn_i in (12) is a linear equation from a double stochastic matrix it arrives to an extremum on the vertices, i.e. the permutation matrices. From this it follows that the maximum final occupation number in a fixed mode is

$$n_k(\tau) = \max\left(n_j(0)\right), \tag{13}$$

therefore, to make the occupation number of a single mode a macroscopic value we need to already have a macroscopic occupation number in a different mode. In other words, in a closed system a condensed state cannot emerge from linear interactions which keep the mean boson number constant with the given initial conditions (3).

3.2. Maximum work extraction

The work extracted from the system can be found by $W = -\Delta E$. The maximal work available for extraction from a system via linear interactions (Gaussian ergotropy) has been calculated in [16]. It is interesting to see what this value will be with the addition constraints of (3) and of constant mean boson number. In this regime the maximum amount of work that can be extracted from the system corresponds to the minimum of ΔE from M_{ij}. As this is once again a linear equation, similar to the previous section an extremum corresponds to a permutation matrix. Thus, the maximum work extracted equals to

$$W_{max} = \sum_{i=1}^{r} \omega_i \left(n_i(0) - n_{k_i}(0)\right), \tag{14}$$

where $n_{k_i}(0) = n_i(\tau)$ is the sequence $n_i(0)$ in an ascending order.

Let us take r to be a macroscopic number while all $n_i(0)$ are finite and small. If $n_i(0)$ are initially uniformly distributed random variables $n_i(0) \in [0,2\nu]$ and $\omega_i = \frac{i}{r}$ then on average the maximum extracted work will be of order

$$W_{max} \sim \frac{\nu}{r} \sum_{i=1}^{r} i(2i - r) = \frac{\nu r}{6}, \tag{15}$$

i.e. a macroscopic amount of work can be extracted from such system via linear interactions that keep the mean boson number constant.

3.3. Relaxed initial constraints

Now assume the third constraint on the initial state in (3) is relaxed, meaning $\langle a_j^\dagger a_k \rangle = \mu_{jk}$ is not diagonal. Using $\langle a_j^\dagger a_k \rangle^* = \langle a_k^\dagger a_j \rangle$ we find that μ is a Hermitian matrix and from (4) we can write its time evolution

$$\mu(\tau) = U\mu(0)U^\dagger, \tag{16}$$

where $U = S^*$. Then using $n_k = \mu_{kk}$ we can find

$$n_i(\tau) = \sum_{j=1}^{r} M_{ij}{}' \bar{\mu}_j, \tag{17}$$

where $\bar{\mu}_j$ are the eigenvalues of matrix μ and M' is another double stochastic matrix which means that $\bar{\mu}$ majorizes $n_i(\tau)$. Once again we can find the maximum occupation in a single mode and the maximal available work making M' a permutation matrix. This means that the maximum occupation in a single mode is less than or equal to the maximum eigenvalue of matrix μ. This mechanism relies on the fundamentally quantum correlations between the creation and annihilation operators of different modes in the initial state. To have macroscopic eigenvalues while the diagonal values are not macroscopic would require a macroscopic amount of modes r and the matrix to either have macroscopic non-diagonal values (macroscopic quantum correlation) or be non-sparse, i.e. have a macroscopically large amount of finite quantum correlation.

4. Conclusions

Frohlich's mechanism of dynamic Bose-Einstein condensation in biological systems is an underdeveloped topic limited by the experimental technology of its time. I show that the necessity of classical non-linearity in Frohlich's condensation is transformed to a necessity of non-linear evolution in a closed quantum system for a broad class of initial states. The simplest thermodynamic derivation of a BEC in an ideal gas is done using the grand canonical ensemble. It is then assumed that a non-equilibrium state can be brought to a BEC state via coupling it with a thermal bath. An important consequence of my results is that this assumption fails for a linearly coupled thermal bath such as the Caldeira-Leggett model [20, 21]. However, I also show that there is a mechanism for a more relaxed class of initial states where condensation via linear interactions could be achievable. This mechanism requires very large or very long-range quantum correlations in the initial state.

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