Robustness of Wave Functions of Interacting Many Bosons in a Leaky Box

Akira Shimizu* and Takayuki Miyadera

Department of Basic Science, University of Tokyo, Komaba, Meguro-ku, Tokyo 153-8902, Japan

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We study the robustness, against the leakage of bosons, of wave functions of interacting many bosons confined in a finite box by deriving and analyzing a general equation of motion for the reduced density operator. We identify a robust wave function that remains a pure state, whereas other wave functions, such as the Bogoliubov's ground state and the ground state with a fixed number of bosons, evolve into mixed states. Although these states all have the off-diagonal long-range order, and the same energy, we argue that only the robust state is realized as a macroscopic quantum state.

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When a quantum system is subject to perturbations from its environment, most wave functions decohere, and only an exceptional wave function(s) remains pure. For quantum systems with a single degree of freedom ($f = 1$), this robust wave function is a coherent state [1,2]. For example, when a coherent state $|\alpha\rangle$ of single-mode photons passes through an absorptive medium, the final state is also a coherent state $|\alpha'\rangle$, which was attenuated ($|\alpha'| < |\alpha|$) by the absorption [1]. It was also argued that, for a $f = 1$ system, coherent states produce the least entropy in the environment, thus being stable [2]. Since these conclusions are based on analyses of $f = 1$ systems, a natural question is: Are they applicable to macroscopic systems, i.e., to $f \gg 1$ interacting systems? Moreover, we must identify which coherent states are robust, because there are many choices of the coordinate (among many degrees of freedom) by which a coherent state is defined. Furthermore, for massive bosons the superselection rule (SSR) forbids superpositions of states with different numbers of bosons. Hence, we must clarify how coherent states can be compatible with the SSR. The purpose of this Letter is to answer these questions for condensates of interacting many bosons, which (or equivalents of which) are observed in many physical systems such as liquid He [3], quantum Hall [4], excitons [5], and trapped atoms [6]. We also discuss the symmetry breaking in view of the robustness.

We consider many bosons which interact with each other repulsively. We assume that the bosons are confined in a large, but finite, box of volume V, which is placed in a huge room of volume $\mathcal{V} \gg V$, which we call the environment. Suppose that the potential of the walls of the box is not high enough, so that the box and the environment exchange bosons via tunneling processes at a small rate (flux) J. Let $t_{\rm eq}$ denote the time scale after which the total system, the box plus the environment, reaches the equilibrium state. We are not interested in the time region $t \geq t_{\rm eq}$ because the equilibrium state is just a uniform state that is determined solely by the initial state of the environment (because $\mathcal{V} \gg V$). We therefore examine the *transient region* for which $t \ll t_{\rm eq}$, in order to discuss the robustness of an initial state $|\phi(0)\rangle$, which is prepared at $t = 0$, of the box. Depending on the choice of the initial state $|\phi_{\rm E}(0)\rangle_{\rm E}$ of the environment, the box state may be affected either drastically or moderately. For example, a moderate situation is that $|\phi_{\rm E}(0)\rangle_{\rm E}$ has the same density n of bosons as $|\phi(0)\rangle$. In such a case, n of the box will be kept constant for all t. To discuss the robustness, however, we consider the severest situation, where the environment is initially in the vacuum state $|0\rangle_{\rm E}$ of bosons, so that bosons escape from the box continuously. If a box state is robust in this severest case, it would also be robust in other cases. Hence, the total wave function at $t = 0$ is $|\Phi(0)\rangle_{\rm total} = |\phi(0)\rangle \otimes |0\rangle_{\rm E}$. We decompose (the $\mathbf{r}$ dependence of) the boson field that is defined on $V + \mathcal{V}$ as $\hat\psi_{\rm total}(\mathbf{r}) = \hat\psi(\mathbf{r}) + \hat\psi_{\rm E}(\mathbf{r})$. Here, $\hat\psi(\mathbf{r})$ localizes in the box, whereas the low-energy component of $\hat\psi_{\rm E}(\mathbf{r})$ localizes in the environment [7]. Accordingly, the Hamiltonian of the total system is decomposed as $\hat H_{\rm total} = \hat H + \hat H_{\rm E} + \hat H_{\rm SE}$. Here, $\hat H$ ($\hat H_{\rm E}$) is a function of $\hat\psi$ ($\hat\psi_{\rm E}$) only, describing interacting bosons in the box (environment). On the other hand, $\hat H_{\rm SE}$ includes both $\hat\psi$ and $\hat\psi_{\rm E}$, describing the $\hat\psi$-$\hat\psi_{\rm E}$ interaction. If the leakage flux J is small, the probability of finding two or more bosons simultaneously in a wall of the box is negligible, and thus the dominant term of $\hat H_{\rm SE}$ takes the following form:

$$\hat H_{\rm SE} = \lambda \int d^3\mathbf{r}\, \hat\psi_{\rm E}^\dagger(\mathbf{r}) w(\mathbf{r}) \hat\psi(\mathbf{r}) + {\rm H.c.} \qquad (1)$$

Here, $w(\mathbf{r})$ represents the shapes of the walls ($w \sim 1$ in the walls, $w = 0$ in other regions), whose potential height is characterized by a parameter λ. Details of w are irrelevant because they are all absorbed in the value of j [Eq. (9) below]. In the time region of interest ($t \ll t_{\rm eq}$), the $\hat\psi_{\rm E}$-$\hat\psi_{\rm E}$ interaction should be unimportant because n of the environment remains zero. On the other hand, we must treat the $\hat\psi$-$\hat\psi$ interaction appropriately. For this purpose, we use the decomposition formula for $\hat\psi$ [8–10]:

$$\hat\psi = \hat\Xi + \hat\psi', \qquad (2)$$

where $\hat\Xi$ is an operator satisfying

$$\hat\Xi|N,G\rangle = \sqrt{N}\,\xi|N-1,G\rangle, \qquad (3)$$

where $|N, G\rangle$ denotes the ground state that has *exactly* N bosons [8,9,11], which we call the number state of interacting bosons (NSIB), and

$$\xi \equiv \langle N - 1, G|\hat{\psi}|N, G\rangle/\sqrt{N} \quad (4)$$

is a hallmark of the condensation: $\sqrt{N}\,\xi = \mathcal{O}(1)$ for condensed states, whereas $\sqrt{N}\,\xi = \mathcal{O}(1/\sqrt{V})$ for normal states [8,9,12]. We here consider the condensed states. Since $\hat{\psi}$ alters N exactly by 1, Eq. (4) means that $\langle N - \Delta N, G|\hat{\psi}|N, G\rangle = \sqrt{N}\,\xi\,\delta_{\Delta N,1}$ for all ΔN such that $|\Delta N| \ll N$. It then follows from Eqs. (2) and (3) that

$$\langle N - \Delta N, G|\hat{\psi}'|N, G\rangle = 0 \quad (\text{for } |\Delta N| \ll N). \quad (5)$$

Namely, $\hat{\psi}'$ transforms $|N, G\rangle$ into excited states.

For weakly interacting bosons, the explicit forms of the NSIB were given in Refs. [9,11], and that of $\hat{\Xi}$ was given in [9]. Because of the boson-boson interaction, they are rather complicated functions of bare operators $\hat{a}_{\mathbf{k}}$: $|N, G\rangle = (1/\sqrt{N!})e^{i\hat{G}}(\hat{a}_0^\dagger)^N|0\rangle$ and $\hat{\Xi} = e^{i\varphi}\sqrt{n_0/nV}\,e^{i\hat{G}}\hat{a}_0 e^{-i\hat{G}}$. Here, $n_0 = \langle \hat{N} - \int d^3\mathbf{r}\,\hat{\psi}'^\dagger\hat{\psi}'\rangle/V$, $\hat{G} \equiv (-i/2nV)\hat{a}_0^\dagger\hat{a}_0^\dagger\sum_{\mathbf{q}\neq\mathbf{0}} y_q\hat{a}_{\mathbf{q}}\hat{a}_{-\mathbf{q}} +$ H.c., φ is an arbitrary phase, and y_q is given in Ref. [9]. By using these expressions, we can show that [10]

$$[\hat{\Xi}, \hat{\Xi}^\dagger],\ [\hat{\Xi}, \hat{\psi}'],\ [\hat{\Xi}, \hat{\psi}'^\dagger] = \mathcal{O}(1/V). \quad (6)$$

Lifshitz and Pitaevskii (LP) [8] claimed that Eq. (6) is applicable even when the interaction is stronger. Their discussion is somewhat controversial because LP started from, instead of Eq. (3), the assumption that $\hat{\Xi}$ could be defined by $\hat{\Xi}|N, \nu\rangle = \Xi|N - 1, \nu\rangle$, where $|N, \nu\rangle$ denotes *any* eigenstate that has exactly N bosons. However, we note that for weakly interacting bosons we have not used this assumption in the derivation of Eq. (6). We thus expect that Eq. (6) also holds for bosons with stronger interaction, even if LP's assumption is too strong. If this is the case, the following results are applicable not only to weakly interacting bosons but also to bosons with stronger interaction, because the results will be derived only from Eqs. (1)–(6).

Since we are studying the robustness against *weak* perturbations, we assume that λ is small, so that J is very small. In this case, we have to consider transitions only among $|N, G\rangle$'s with different N's (i.e., we can neglect transitions to excited states). Hence, the reduced density operator $\hat{\rho}$ can be generally written as

$$\hat{\rho}(t) = \sum_{N,M} \rho_{NM}(t)|N, G\rangle\langle M, G|. \quad (7)$$

It seems almost obvious that quantum coherence between $|N, G\rangle$ and $|M, G\rangle$ with large $|N - M|$ would be destroyed by the interaction with the environment. We therefore study the most interesting case, where ρ_{NM} is localized in the N-M plane in such a way that $\sqrt{\langle\delta N^2\rangle} \ll \langle N\rangle$. If this relation is satisfied at $t = 0$, it is also satisfied for all $t \ll t_{\mathrm{eq}}$. We also assume that $\mathcal{V}$ is large enough, so that the boson density in the environment $(= [\langle N(0)\rangle - \langle N(t)\rangle]/\mathcal{V})$ is negligibly small for all $t \ll t_{\mathrm{eq}}$. Under these conditions, we can calculate the time evolution of $\rho_{NM}(t)$, using Eqs. (1)–(6), as [10,13]

$$\rho_{NM}(t + \Delta t) = e^{-i(N-M)\mu(n(t))\Delta t/\hbar} \times \{\rho_{NM}(t)[1 - (N + M)j(n(t))\Delta t/2] + \rho_{N+1,M+1}(t)\sqrt{(N + 1)(M + 1)}\,j(n(t))\Delta t\} + \mathcal{O}(\lambda^4), \quad (8)$$

for a finite time interval Δt that satisfies $\hbar/E_c \lesssim \Delta t < 1/\langle N\rangle j(n)$, where E_c is the energy scale over which the matrix elements of $\hat{H}_{\mathrm{SE}}$ are non-negligible. Here, $n \equiv \langle N\rangle/V$, and $\mu(n)$ (>0 for a condensate of interacting bosons [3,8,9]) denotes the chemical potential of bosons in the box. Furthermore,

$$j(n) = K\,\frac{2\pi}{\hbar}\,\frac{n_0}{n}\,|\lambda|^2\,\frac{v^2}{V}\,D(\mu(n)), \quad (9)$$

where $D(\mu)$ is the density of states per unit volume of the environment at energy μ, v is the total volume of the walls of the box, and K is a constant of order unity. Both μ and j depend on $\langle N\rangle$ through n, but this dependence is very weak because a change of $\langle N\rangle$ by 1 only causes the change of n by $1/V$. Note that our basic equation (8) has only two parameters, μ and j. Namely, all model-dependent parameters (details of $\hat{H}$, $\hat{H}_{\mathrm{E}}$, and $\hat{H}_{\mathrm{SE}}$) are absorbed in these two parameters. Therefore, the following results are general and model independent.

Using Eq. (8), we first calculate the time evolutions of the expectation value $\langle N\rangle$ and the fluctuation $\langle\delta N^2\rangle$ of the number N of bosons in the box. We find

$$\frac{d}{dt}\langle N\rangle = -j(n)\langle N\rangle. \quad (10)$$

Hence, $\langle N\rangle$ decreases gradually because of the leakage flux $J = j(n)\langle N\rangle$. For $\langle\delta N^2\rangle$, on the other hand, we find

$$\frac{d}{dt}F = j(n)[1 - F], \quad (11)$$

where $F \equiv \langle\delta N^2\rangle/\langle N\rangle$ is the "Fano factor" [1]. It is seen that a robust state must have $F = 1$, whereas any states with $F \neq 1$ are fragile in the sense that their F evolves with time, approaching unity. For example, the ground-state wave function in the Bogoliubov approximation, $|\mathrm{Bog}, G\rangle$, has $F > 1$ [9]. Hence, it is fragile. The ground-state wave function with a fixed number of bosons, $|N, G\rangle$, is also fragile because $F = 0$.

Since the evaluation of F is easy, F is a convenient tool for the investigation of the robustness. However, since

F is only related to the diagonal elements of $\hat{\rho}$, it does not distinguish between pure and mixed states. Therefore, we now solve the basic equation (8) for various initial states to investigate the robustness of the wave functions in more detail. When the initial state is a pure state of the NSIB, i.e., $\hat{\rho}(0) = |N, G\rangle\langle N, G|$, then ρ_{NM} after a short interval Δt is evaluated as $\rho_{NN}(\Delta t) = [1 - Nj(n(t))\Delta t]$, $\rho_{N-1,N-1}(\Delta t) = Nj(n(t))\Delta t$, and other elements are zero. Therefore, $\hat{\rho}$ becomes a classical mixture of $|N, G\rangle$ and $|N - 1, G\rangle$ at $t = \Delta t$, consistent with the above result that shows that states with $F = 0$ are fragile. By evaluating the evolution at later times, we find that $\hat{\rho}$ evolves toward a Poissonian mixture of $|N, G\rangle$'s [13], consistent with $F \to 1$. In a similar manner, we can show that the pure state of Bogoliubov's ground state $\hat{\rho}(0) = |\mathrm{Bog}, G\rangle\langle \mathrm{Bog}, G|$, which has $F > 1$, also evolves into a mixed state. We can also show that the number-phase squeezed state of interacting bosons (NPIB), which was found in Ref. [9] as a number-phase minimum uncertainty state with $0 < F < 1$, also evolves into a mixed state. These examples show that F is indeed a simple measure of the robustness: A pure state with $F \neq 1$ is unlikely to remain pure. Note, however, that a pure state with $F = 1$ is not necessarily robust. For example, we can show that the coherent state of free bosons (CSFB) evolves into a mixed state, although it has $F = 1$. Hence, $F = 1$ is only a *necessary condition* for the robustness.

Among many states with $F = 1$, we have successfully found a very special state that is robust in the sense that it remains pure when it is weakly perturbed by the environment. The state is given by

$$\hat{\rho}(t) = |\alpha(t), G\rangle\langle\alpha(t), G|. \tag{12}$$

Here, $\alpha(t)$ is a time-dependent complex number given by

$$\alpha(t) = e^{i\varphi(t)}\sqrt{\langle N(t)\rangle}, \tag{13}$$

where $\langle N(t)\rangle$ is the solution of Eq. (10), and

$$\varphi(t) = \varphi(0) - \frac{i}{\hbar}\int_0^t \mu(n(t))\,dt. \tag{14}$$

Here, the initial phase $\varphi(0)$ is arbitrary, and $n(t) \equiv \langle N(t)\rangle/V$. Furthermore,

$$|\alpha, G\rangle \equiv e^{-|\alpha|^2/2}\sum_{M=0}^{\infty}\frac{\alpha^M}{\sqrt{M!}}|M, G\rangle, \tag{15}$$

which we call the coherent state of interacting bosons (CSIB). It has the same form as the CSFB, except that $|M, G\rangle$ is the NSIB. Because of this difference, simple relations for the CSFB do not hold for the CSIB. For example, $\langle\alpha, G|\hat{\psi}|\alpha, G\rangle \neq \alpha/\sqrt{V}$, and, moreover, $|\alpha, G\rangle$ is not an eigenstate of $\hat{\psi}$. Nevertheless, $\langle\alpha, G|\hat{N}|\alpha, G\rangle = \langle\alpha, G|\delta\hat{N}^2|\alpha, G\rangle = |\alpha|^2$, hence $F = 1$ exactly, as in the case of CSFB. Since the NSIB has a complicated wave function, so does the CSIB. (For weakly interacting bosons, its explicit form was given in Ref. [9].) Although complicated, the wave function of the CSIB is robust against weak perturbations from the environment: It keeps the same form, whose parameter $\alpha(t)$ evolves slowly (except for the phase rotation), and remains a pure state, in contrast to other wave functions which soon evolve into mixed states. In fact, Eqs. (12)–(15) yield

$$\rho_{NM}(t) = e^{-\langle N(t)\rangle}\frac{e^{i(N-M)\varphi}}{\sqrt{N!M!}}\langle N(t)\rangle^{(N+M/2)}, \tag{16}$$

$$\rho_{NM}(t + \Delta t) = e^{-\langle N(t)\rangle(1-j\Delta t)}\frac{e^{i(N-M)(\varphi-\mu\Delta t/\hbar)}}{\sqrt{N!\,M!}} \times \langle N(t)\rangle^{(N+M/2)}(1 - j\Delta t)^{(N+M/2)}, \tag{17}$$

which indeed satisfy Eq. (8).

We now discuss the compatibility with the SSR, which might raise the objection that the CSIB would not be realized because superpositions between states with different values of N are forbidden for massive bosons. To show that this intuitive objection is wrong, it is sufficient to give one counterexample. Suppose that there is another box, which also contains condensed bosons, in the same room. The total system consists of two boxes and the environment. According to the SSR, the wave function of the total system $|\Phi\rangle_{\mathrm{total}}$ should be a superposition of states that have the same number of bosons, $N_{\mathrm{total}} = N + N' + N_{\mathrm{E}} =$ fixed, where N' denotes the number of bosons in the second box. Consider the following state, which satisfies this constriction:

$$|\Phi\rangle_{\mathrm{total}} = \sum_{N,N',\ell} e^{-|\alpha|^2/2-|\alpha'|^2/2}\alpha^N\alpha'^{N'}C_\ell/\sqrt{N!\,N'!} \times |N, G\rangle \otimes |N', G\rangle' \otimes |N_{\mathrm{total}} - N - N', \ell\rangle_{\mathrm{E}}. \tag{18}$$

Here, $\alpha = |\alpha|e^{i\varphi}$, $\alpha' = |\alpha'|e^{i\varphi'}$, and C_ℓ is a complex number, where ℓ is a quantum number labeling states of the environment $|M, \ell\rangle_{\mathrm{E}}$ which has M bosons. Regarding the phases φ and φ', only the relative value $\varphi - \varphi' \equiv \theta$ has a physical meaning. We thus take $\varphi' = 0$ henceforth. Equation (18) yields the reduced density operator of the first box as $\hat{\rho} = \sum_N e^{-|\alpha|^2}(|\alpha|^{2N}/N!)\,|N, G\rangle\langle N, G|$. It is easy to show that this is identical to

$$\hat{\rho} = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\,||\alpha|e^{i\theta}, G\rangle\langle|\alpha|e^{i\theta}, G|. \tag{19}$$

Although this $\hat{\rho}$ represents a mixed state of CSIB's, we note that *it does not contain the maximum information* on the state in the box, whereas the best density operator should have the maximum information. The lacking information is that the phase relative to the condensate in the second box is φ. Hence, the maximum information is Eq. (19) with the restriction $\theta = \varphi$.

This combined information is concisely expressed as $\hat{\rho} = ||\alpha|e^{i\varphi}, G\rangle\langle|\alpha|e^{i\varphi}, G|$, which agrees with Eq. (12). Namely, Eq. (12) is better than Eq. (19) because it contains more information. This example demonstrates that Eq. (12) can be compatible with the SSR in realistic cases where the box exchanges bosons with the environment. Only in the limiting case where the box is completely closed should the SSR be crucial, and the NSIB would be realized if the temperature $T \to 0$ [14].

We have established that the CSIB is a robust pure state of interacting many bosons. We finally discuss its implications. The robustness of the present work should not be confused with the "stiffness of macroscopic wave functions" [3,4], which refers only to the stability of an order parameter in a mean field approximation. For example, $|\mathrm{Bog}, G\rangle$ has the stiffness [3,4], whereas it is fragile as we have shown. The robustness is a generalization of the robustness of coherent states of $f = 1$ systems [1,2]. It is thus natural to expect that, for $f \gg 1$ systems, *some* coherent state would be robust. However, it was not known *which* coherent state is robust: there are many choices of the coordinate by which a coherent state is defined. Since Eq. (3) yields

$$(\hat{\Xi}/\xi)|\alpha, G\rangle = \alpha|\alpha, G\rangle, \tag{20}$$

this work has revealed that the robust coherent state is the one defined by $\hat{\Xi}/\xi$. In this sense, $\hat{\Xi} + \hat{\Xi}^\dagger$ is the "natural coordinate" of interacting many bosons. The condensation of bosons are often characterized by the off-diagonal long-range order (ODLRO) that is defined by $\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle =$ finite for $|\mathbf{r} - \mathbf{r}'| \sim V^{1/3}$. By using Eqs. (2)–(5) we can show that the CSIB, NSIB, NPIB, and the Bogoliubov's ground state all have the ODLRO. Hence, the present work has revealed that the ODLRO does not necessarily imply the robustness. Furthermore, all of these states have the same energy, i.e., the differences of $\langle\hat{H}\rangle$ are only $\mathcal{O}(1/V)$ for the same value of $\langle N\rangle$ [15]. For example, if we let $E_{N,G}$ be the eigenenergy of the NSIB, $\hat{H}|N, G\rangle = E_{N,G}|N, G\rangle$, we can then easily show from Eq. (15), that, by neglecting terms of $\mathcal{O}(1/V)$, $\langle\alpha, G|\hat{H}|\alpha, G\rangle = E_{|\alpha|^2,G} = E_{\langle N\rangle,G}$. Therefore, the robustness of the CSIB is *not* due to an energy difference, but to natures of wave functions. Since interactions with the environment are finite in most physical systems, we argue that only the robust state, CSIB, should be realized as a macroscopic pure state. Since the (relative) phase of the CSIB is almost definite [9], the global gauge symmetry is then broken. Although V is finite, we are thus led to the symmetry breaking by considering the robustness. This suggests that quantum phase transitions may have more profound origins than singularities that are developed as $V \to \infty$. A conventional trick to get symmetry breaking states for boson condensates is to introduce a symmetry breaking field η, which couples to $\hat{\psi}$ as $\hat{H}_\eta = \int d^3\mathbf{r}\,(\eta^*\hat{\psi} + \eta\hat{\psi}^\dagger)$. However, η is usually considered as an unphysical field [3,16,17], and it was sometimes argued that symmetry breaking states were meaningless because they look against the SSR [17]. In contrast, this paper gives a physical reasoning for the symmetry breaking, assuming only physical interactions, and shows the compatibility with the SSR.

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*Electronic address: shmz@ASone.c.u-tokyo.ac.jp

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