Energies and collapse times of symmetric and symmetry-breaking states of finite systems with a U(1) symmetry

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We study quantum systems of volume V, which will exhibit the breaking of a U(1) symmetry in the limit of $V\to\infty$, when V is large but finite. We estimate the energy difference between the ''symmetric ground state'' (SGS), which is the lowest-energy state that does not break the symmetry, and a ''pure phase vacuum'' (PPV), which approaches a symmetry-breaking vacuum as $V\to\infty$. Under some natural postulates on the energy of the SGS, it is shown that PPVs always have a higher energy than the SGS, and we derive a lower bound of the excess energy. We argue that the lower bound is $O(V^0)$, which becomes *much larger* than the excitation energies of low-lying excited states for a large V. We also discuss the collapse time of PPVs for interacting many bosons. It is shown that the wave function collapses in a microscopic time scale, because PPVs are not energy eigenstates. We show, however, that for PPVs the expectation value of any observable, which is a finite polynomial of boson operators and their derivatives, does not collapse for a macroscopic time scale. In this sense, the collapse time of PPVs is macroscopically long.

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The symmetry breaking (SB) is a key to understand quantum systems of many degrees of freedom. Although SB is *formally* defined for infinite systems, the physics of SBs in *finite* systems have been attracting much attention [1–8] for the following reasons.

(i) Progress of experimental techniques enables one to observe and examine phase transitions in small systems, such as small magnets, small superconductors [9], liquid Helium in a small bubble [10], and laser-trapped atoms [11], hence SBs in finite systems should be studied seriously.

(ii) Although recent progress of computers enables one to obtain ground states of finite systems numerically, the relation between such ground states and SB ground states of *infinite* systems are nontrivial.

In a mean-field approximation, ground states of a finite system of volume V are degenerate (if it will exhibit a SB as $V\to\infty$), and each ground state approaches a SB vacuum of the infinite system as $V\to\infty$. We call such a state that has a finite expectation value of an order parameter and approaches (i.e., well approximates) a SB vacuum of the infinite system as $V\to\infty$ a ''pure phase vacuum'' (PPV). On the other hand, if one diagonalizes the Hamiltonian of the finite system exactly, the energy spectrum is much different from that of a mean-field approximation. The ground states are not necessarily degenerate. Moreover, it often occurs that a symmetric state that does not break the symmetry is a ground state, whereas PPVs have higher energies [1–7], in the absence of a SB field, which is usually considered as an unphysical, artificial field for the breaking of a U(1) symmetry. We call such a ground state the ''symmetric ground state'' (SGS). In contrast to PPVs, the SGS does not approach a SB vacuum of the infinite system as $V\to\infty$. Hence, for a SB to occur, the energy difference between PPVs and the SGS should be small enough. Although the magnitude of this energy difference has been attracting much attention [1–7], definite conclusions have not yet been reached for the breaking of a U(1) symmetry. For example, an exact calculation [5] gave only a rough estimate [see the discussion following Eq. (15)].

In this paper, we estimate much more strictly the energy difference between PPVs and the SGS for the breaking of a U(1) symmetry. Under some natural postulates on the energy of the SGS, we show that PPVs always have a higher energy than the SGS, and that the excess energy is lower bounded by $\mu'\langle\delta N^2\rangle/2V$, where μ' is the derivative of the chemical potential with respect to the density $n\equiv\langle N\rangle/V$, and $\langle\delta N^2\rangle$ denotes the fluctuation of 'charge' N. We further argue that this lower bound is $O(V^0)$, which becomes *much larger* than the excitation energies of low-lying excited states for a large V. This should be contrasted with the breaking of the $\mathbf{Z}_2$ symmetry, for which the energy difference between PPVs and the SGS is only $O(V^{-1})$ [1], which becomes *much smaller* than the excitation energies in a three-dimensional space for a large V. We also study the collapse time $t_{\rm coll}$ of PPVs for the case of interacting many bosons. It is shown that $t_{\rm coll}=O(V^0)$ for the wave function, because PPVs are not energy eigenstates. We show, however, that for PPVs $t_{\rm coll}=O(\sqrt{V})$ for the expectation value of any observable, which is a finite polynomial of boson operators and their derivatives, if the degree of the polynomial is fixed independent of V. In this sense, the collapse time of PPVs is macroscopically long.

We consider a quantum system that has a U(1) symmetry, whose conserved charge $\hat{N}$ has integral eigenvalues (in an appropriate unit). We assume that the system is uniform, with the periodic boundary conditions, in order to eliminate additional complexities caused by nonuniform potentials or surface effects. Since the system volume V is finite, $\hat{N}$ is always well defined, hence there exist simultaneous eigenstates $|N,\ell\rangle$ of $\hat{H}$ and $\hat{N}$;

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$$\hat{H}|N,\ell\rangle = E_{N,\ell}|N,\ell\rangle, \tag{1}$$

$$\hat{N}|N,\ell\rangle = N|N,\ell\rangle, \tag{2}$$

where ℓ is a (set of) quantum number(s). For each value of N, there exists the lowest-energy state $|N,G\rangle$, which we assume is nondegenerate. In general, $\hat{N}$ becomes the generator of the U(1) symmetry. Hence, $|N,G\rangle$ is the SGS. We now make two basic postulates: postulate 1 is the extensivity of the lowest eigenenergy,

$$E_{N,\mathrm{G}} = V\epsilon(N/V), \tag{3}$$

where ϵ is a single-variable function of the charge density N/V. This postulate seems natural under our assumptions that the system is uniform and $|N,G\rangle$ is nondegenerate, as long as the charge does not induce a long-range force. (Hence, care must be taken when the present results are applied to systems for which N is the electric charge.) By taking the limit $V\to\infty$, we can define $\epsilon(n)$ for every continuous value of $n(=N/V)$. Using this $\epsilon(n)$ for a finite V as well, we can regard N in Eq. (3) as a continuous variable. Hence, we can define $\mu(n)\equiv\epsilon'(n)=(\partial/\partial N)E_{N,G}$. Postulate 2 is

$$\mu'(n)\equiv\epsilon''(n)=V\frac{\partial^2}{\partial N^2}E_{N,G}>0, \tag{4}$$

which also seems natural because thermodynamics requires that μ should be a nondecreasing function of n, for the system to be stable. Although $\mu'=0$ for noninteracting particles (such as a photon gas whose μ is always zero), we assume $\mu'>0$ because we are not interested in such a trivial case. For weakly interacting many bosons with a repulsive interaction (with the effective coupling constant $g>0$), for example, these postulates are indeed satisfied, $E_{N,\mathrm{G}}=V\epsilon(N/V)$, where $\epsilon(n)=gn^2/2+\cdots$, hence $\mu'=g+\cdots>0$.

When the system exhibits the breaking of the U(1) symmetry in the limit of $V\to\infty$ (while keeping the charge density finite), a SB state cannot be $\lim_{V\to\infty}|N,G\rangle$ or $\lim_{V\to\infty}|N,\ell\rangle$, because they are eigenstates of $\hat{N}$ [1–7]. Therefore, one should take superpositions of states with different charges in order to construct a PPV, which approaches (i.e., well approximates) a SB vacuum as $V\to\infty$ [1–7]. If the quantum system (of a finite V) is perfectly closed, such superpositions are forbidden for massive and/or charged particles by the charge superselection rule, which requires that any pure state must be an eigenstate of $\hat{N}$ [12]. However, if the quantum system is a subsystem of a larger system [13], we previously showed that one can associate a pure state, which is a coherent superposition of states with different charges, to the subsystem [6,14]. We investigate energy expectation values of such states, which in general have either of the following forms;

$$|C\rangle \equiv \sum_N C_N|N,G\rangle, \tag{5}$$

$$|\tilde{C}\rangle \equiv \sum_{N,\ell} \tilde{C}_{N,\ell}|N,\ell\rangle, \tag{6}$$

where C_N and $\tilde{C}_{N,\ell}$ are coefficients, which are normalized as $\Sigma_N|C_N|^2=1$ and $\Sigma_{N,\ell}|\tilde{C}_{N,\ell}|^2=1$, respectively. We are interested in the case where the charge density $n(=\langle N\rangle/V)$ approaches a finite value as $V\to\infty$. (On the other hand, the case $n\to 0$ is rather trivial, while the case $n\to\infty$ is anomalous.) Namely,

$$\langle N\rangle = O(V), \tag{7}$$

where $\langle N\rangle\equiv\langle C|\hat{N}|C\rangle$ or $\langle\tilde{C}|\hat{N}|\tilde{C}\rangle$, and $n=\langle N\rangle/V$. Furthermore, PPVs should be consistent with thermodynamics, according to which variances of extensive variables are of $O(V)$ or smaller. Hence,

$$\langle\delta N^2\rangle \leqslant O(V), \tag{8}$$

where $\langle\delta N^2\rangle\equiv\langle C|\delta\hat{N}^2|C\rangle$ or $\langle\tilde{C}|\delta\hat{N}^2|\tilde{C}\rangle$, where $\delta\hat{N}\equiv\hat{N}-\langle N\rangle$. Namely, C_N and $\tilde{C}_{N,\ell}$ should localize in the N space in such a way that Eqs. (7) and (8) are satisfied. Note that the phases of C_N and $\tilde{C}_{N,\ell}$ are irrelevant to $\langle N\rangle$, $\langle\delta N^2\rangle$, and to the energy expectation values, $\langle C|\hat{H}|C\rangle=\Sigma_N|C_N|^2E_{N,\mathrm{G}}$ and $\langle\tilde{C}|\hat{H}|\tilde{C}\rangle=\Sigma_{N,\ell}|C_N|^2E_{N,\ell}$.

For $N=\langle N\rangle+\Delta N$, where $(\Delta N)^2\leqslant O(V)$, Eq. (3) can be expanded as

$$E_{N,\mathrm{G}}=V\left[\epsilon\left(\frac{\langle N\rangle}{V}\right)+\frac{\Delta N}{V}\mu\left(\frac{\langle N\rangle}{V}\right)+\frac{1}{2}\left(\frac{\Delta N}{V}\right)^2\mu'\left(\frac{\langle N\rangle}{V}\right)+O\left(\frac{1}{V^{3/2}}\right)\right]. \tag{9}$$

We neglect the higher-order term, $VO(1/V^{3/2})$, in the following analysis. Then, we can easily show that

$$\langle C|\hat{H}|C\rangle = E_{\langle N\rangle,\mathrm{G}}+\frac{\langle\delta N^2\rangle}{2V}\mu'\left(\frac{\langle N\rangle}{V}\right). \tag{10}$$

Since the last term is positive because of postulate 2, we conclude that $|C\rangle$ *always has a higher energy than* $|N,G\rangle$ *if they have the same value of* $\langle N\rangle$. Here, it is crucial to fix the value of $\langle N\rangle$ for the comparison. [Otherwise, either state could have a higher energy because of the linear term in Eq. (9).] Note that formula (10), although very simple, gives the energy of a general state of the form (5) very precisely, with the error being only $O(1/V^{1/2})$. Note also that the energy expectation value is determined only by $\langle N\rangle$ and $\langle\delta N^2\rangle$ if the functional forms of $E_{N,\mathrm{G}}$ and $\mu'(n)$ are given.

For a more general state (6), we derive an inequality. Let C'_N's be some coefficients that satisfy $|C'_N|^2=\Sigma_\ell|\tilde{C}_{N,\ell}|^2$. For $|C'\rangle\equiv\Sigma_N C'_N|N,G\rangle$,

$$\langle\tilde{C}|\hat{H}|\tilde{C}\rangle-\langle C'|\hat{H}|C'\rangle=\sum_{N,\ell}|\tilde{C}_{N,\ell}|^2(E_{N,\ell}-E_{N,G})\geqslant 0, \tag{11}$$

where the equality holds iff $\tilde{C}_{N,\ell}=0$ for all $\ell \neq \mathrm{G}$. Applying Eq. (10) to $\langle C'|\hat{H}|C'\rangle$, and noting that $\langle \tilde{C}|\hat{N}|\tilde{C}\rangle = \langle C'|\hat{N}|C'\rangle$ and $\langle \tilde{C}|\delta\hat{N}^2|\tilde{C}\rangle = \langle C'|\delta\hat{N}^2|C'\rangle$, we obtain

$$\langle \tilde{C}|\hat{H}|\tilde{C}\rangle \geq E_{\langle N\rangle,G} + \frac{\langle \delta N^2\rangle}{2V}\mu'\left(\frac{\langle N\rangle}{V}\right). \tag{12}$$

When $|\tilde{C}\rangle$ and $|C\rangle$ have the same values of $\langle N\rangle$ and $\langle \delta N^2\rangle$, Eqs. (10) and (12) can be combined as the simple formula,

$$\langle \tilde{C}|\hat{H}|\tilde{C}\rangle \geq \langle C|\hat{H}|C\rangle = E_{\langle N\rangle,G} + \frac{\langle \delta N^2\rangle}{2V}\mu'\left(\frac{\langle N\rangle}{V}\right). \tag{13}$$

It is easy to show a similar result for $\hat{K}\equiv\hat{H}-\mu\hat{N}$, where μ here is a constant,

$$\langle \tilde{C}|\hat{K}|\tilde{C}\rangle \geq \langle C|\hat{K}|C\rangle = K_{\langle N\rangle,\mathrm{G}} + \frac{\langle \delta N^2\rangle}{2V}\epsilon''\left(\frac{\langle N\rangle}{V}\right), \tag{14}$$

where $K_{N,G}\equiv E_{N,G}-\mu N$. Hence, the following results are applicable to the expectation values of $\hat{K}$ as well, if we replace $K_{N,G}$ and μ' with $E_{N,G}$ and ϵ'', respectively.

Since a PPV should take either form (5) or (6), we conclude that (i) a PPV always has a higher energy than the SGS, and (ii) the excess energy is lower bounded by $\mu'\langle \delta N^2\rangle/2V$. This is the first of the main results of this paper. It should be mentioned that Ref. [5] tried to give an *upper* bound of the energy *difference* between the SGS and ''low-lying states,'' a linear combination of which is a PPV, while our result gives a *lower* bound of the energy *increase* of PPVs over the SGS.

We now estimate how the lower bound $\mu'\langle \delta N^2\rangle/2V$ behaves with increasing V. For interacting many bosons, we previously found the state vector of a PPV, which we called the coherent state of interacting bosons (CSIB) [6,7,15]. This state vector, denoted by $|\alpha,G\rangle$, has the form of Eq. (5) with $C_N=e^{-|\alpha|^2}\alpha^N/\sqrt{N!}$. Hence, $\langle \delta N^2\rangle=\langle N\rangle$, and Eq. (10) yields

$$\langle \alpha,G|\hat{H}|\alpha,G\rangle - E_{\langle N\rangle,G} = (n/2)\mu'(n) = O(V^0) > 0, \tag{15}$$

where the sign is determined by postulate 2($\mu'>0$), and $n=\langle N\rangle/V$. On the other hand, if we apply the inequality of Ref. [5] to the CSIB, we obtain $|\langle \alpha,G|\hat{H}|\alpha,G\rangle - E_{\langle N\rangle,G}| \leq O(\sqrt{V})$, which diverges as $V\to\infty$. Although there is no contradiction between the two results, the present result gives a much more accurate estimate. The CSIB has a higher energy than the SGS by $O(V^0)$, for the same value of $\langle N\rangle$. Although one might expect that the energy increase would be a decreasing function of V (as in the case of the breaking of the $\mathbf{Z}_2$ symmetry [1]), our result denies such a naive expectation.

For general systems that exhibit the breaking of a U(1) symmetry, we do not know the explicit forms of PPVs. By virtue of relation (13), however, it is sufficient to estimate $\langle \delta N^2\rangle$ for the estimation of the energy increase. We argue that

$$\langle \delta N^2\rangle \sim \langle N\rangle \tag{16}$$

for general systems that exhibit the breaking of a U(1) symmetry, for the following reason. Macroscopic properties of PPVs must be stable against weak perturbations from environments. The environments include those which exchange charges with the system. We may apply the classical stochastic theory to estimate the stable distribution of the charges because (i) the phases of C_N and $\tilde{C}_{N,\ell}$ are irrelevant to $\langle N\rangle$ and $\langle \delta N^2\rangle$, and (ii) the phase coherence between the environments and the system may be negligible if the dephasing times of the environments are short enough. Then, according to the classical stochastic theory, the steady-state distribution of the charges should satisfy Eq. (16) when charges are randomly exchanged with a huge environment.

From Eqs. (4), (7), (13), and (16), we obtain

$$\langle \mathrm{PPV}|\hat{H}|\mathrm{PPV}\rangle - E_{\langle N\rangle,\mathrm{G}} \geq O(V^0) > 0, \tag{17}$$

for general systems that exhibit the breaking of a U(1) symmetry. Note that this result is consistent with the theory of SBs in *infinite* systems, according to which PPVs have the same energy *density* as the SGS [16]. In fact, Eq. (17) yields $(\langle \mathrm{PPV}|\hat{H}|\mathrm{PPV}\rangle - E_{\langle N\rangle,G})/V \geq O(V^{-1}) \to 0$ as $V\to\infty$, for the lower bound of the difference in the energy *densities*. On the other hand, our result denies a naive expectation that the energies of PPVs and the SGS would be ''almost degenerate'' in the sense that the energy difference would be a decreasing function of V. Furthermore, the energy difference for a large V becomes *much larger* than the excitation energies of low-lying excited states, whose wave number $k \propto V^{-1/d}$ in a d-dimensional space, because the excitation energy $\epsilon(k)$ behaves as $\epsilon(k)\propto|k|\propto V^{-1/d}$ for a linear dispersion, and $\epsilon(k)\propto|k|^2=V^{-2/d}$ for a parabolic dispersion. This should be contrasted with the breaking of the $\mathbf{Z}_2$ symmetry, for which the energy difference between PPVs and the SGS is only $O(V^{-1})$ [1], which becomes *much smaller* than the excitation energies in a three-dimensional space for a large V. This indicates, for example, that much more care is necessary for the breaking of the U(1) symmetry than for the breaking of the $\mathbf{Z}_2$ symmetry, when one tries to find a PPV by numerical calculations.

We finally discuss the collapse time of PPVs, by generalizing the discussion of Ref. [8]. In general, PPVs are not an energy eigenstate, hence their wave functions deform in finite systems as time evolves. Let t_{coll} be the *collapse time*, which is defined as the time scale at which this deformation becomes significant. For example, for an initial ($t=0$) state of the form of Eq. (5), it evolves as $|C\rangle \to \sum_N C_N e^{-iE_{N,\mathrm{G}}t}|N,G\rangle \equiv |C;t\rangle$ where $\hbar$ is taken as unity. Since $E_{\langle N\rangle+\Delta N,G}-E_{\langle N\rangle,G}=\mu\Delta N+\cdots$ from Eq. (9), the difference of $|C;t\rangle$ from $|C\rangle$ becomes significant at $t=t_{\mathrm{coll}} \sim 1/\mu\sqrt{\langle \delta N^2\rangle}$, because the linear term $\mu\Delta N$ alters the relative phases among C_N's, except when C_N's take some special forms. As V is increased, this time scale approaches zero if $\sqrt{\langle \delta N^2\rangle}$ increases in proportion to V as Eq. (16). On the other hand, PPVs must survive over a macroscopic time scale, i.e., $t_{\mathrm{coll}}\to\infty$ as $V\to\infty$ for PPVs. To satisfy this condition, C_N's of PPVs must take some special forms. For interacting many bosons, for example, C_N's of the CSIB indeed have special forms, for which the effect of the linear term $\mu \Delta N$ on $|\alpha,G;t\rangle$ is completely absorbed as a time evolution of the single parameter α. In fact,

$$|\alpha,\mathrm{G};t\rangle = e^{-|\alpha|^2}\sum_N \frac{\alpha^N}{\sqrt{N!}} e^{-i[E_{\langle N\rangle,G}+\mu\Delta N+\mu'(\Delta N)^2/2V]t}|N,G\rangle \tag{18}$$

$$= e^{-i(E_{\langle N\rangle,G}-\mu\langle N\rangle)t} e^{-|\alpha|^2}\sum_N \frac{(\alpha e^{-i\mu t})^N}{\sqrt{N!}} \times e^{-i[\mu'(\Delta N)^2/2V]t}|N,G\rangle. \tag{19}$$

Since the prefactor $e^{-i(E_{\langle N\rangle,G}-\mu\langle N\rangle)t}$ has no physical meaning, we find that $|\alpha,G;t\rangle = |\alpha e^{-i\mu t},G\rangle$ if $\mu'=0$. Namely, the CSIB does not collapse at all if $\mu'=0$, only the phase of α evolves with time as $\alpha e^{-i\mu t}$. This result for $\mu'=0$ is well known. If $\mu'>0$, on the other hand, the wave function $|\alpha,G\rangle$ collapses at $t\sim V/\mu'(\Delta N)^2 \sim V/\mu'\langle \delta N^2\rangle = O(V^0)$. However, this does *not* necessarily mean that the expectation values of observables of interest alter in this time scale. For example, if an observable is proportional to the boson operator $\hat{\psi}$ or its derivative, it detects the phase relation between adjacent coefficients, C_{N+1} and C_N. The ratio of their phases evolves, for $N=\langle N\rangle + \Delta N$, as

$$\frac{(e^{-i\mu t})^{N+1} e^{-i\mu'(\Delta N+1)^2 t/2V}}{(e^{-i\mu t})^N e^{-i\mu'(\Delta N)^2 t/2V}} = e^{-i\mu t} e^{-i\mu' t/2V} e^{-i\mu'\Delta N t/V}. \tag{20}$$

In the right-hand side, the first factor $e^{-i\mu t}$ can be absorbed as the time evolution of the single parameter $\alpha \to \alpha e^{-i\mu t}$, whereas the second factor $e^{-i\mu' t/2V}$ is negligible because $\mu'/2V = O(1/V)$. Hence, only the last factor $e^{-i\mu'\Delta N t/V}$ is relevant to the collapse time. We thus find

$$t_{\mathrm{coll}} \sim V/(\mu'\Delta N) \sim V/(\mu'\sqrt{\langle \delta N^2\rangle}) = O(\sqrt{V}). \tag{21}$$

For general observables that are polynomials of degree M of $\hat{\psi}$, $\hat{\psi}^\dagger$ and their derivatives, we obtain

$$t_{\mathrm{coll}} = O(\sqrt{V}/M). \tag{22}$$

Hence, if the degree M of the polynomial is fixed independent of V, we again obtain $t_{\mathrm{coll}} = O(\sqrt{V})$. Since the expectation values of observables are relevant in quantum theory, we may conclude that the collapse time of the CSIB is $O(\sqrt{V})$, which is macroscopic in the sense that it diverges as $V\to\infty$, although the collapse time of its wave function is $O(V^0)$ [17]. If, on the other hand, M is increased in proportion to $\sqrt{V}$, then $t_{\mathrm{coll}} = O(V^0)$. Except for such an abnormal case (as $M \propto \sqrt{V}$), t_{coll} is macroscopic. For more general systems with the breaking of U(1) symmetry, we have not yet obtained definite conclusions on t_{coll}, although we expect a situation similar to the case of interacting many bosons. This may be a subject of future studies.

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[12] See, e.g., R. Haag, *Local Quantum Physics* (Springer, Berlin, 1992).
[13] For example, the trapped BEC systems are not closed because atoms escape from the trap via three-body collisions, dipolar relaxations, and collisions with atoms in background gases. Furthermore, the trapped atoms consist of those in the ground state (BEC), a thermal cloud, and (possibly) outer clouds; collisions among them occur continually.
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[15] The ground state with a definite number of bosons, $|N,G\rangle$, is the SGS that does not approach the correct vacuum of the infinite system as $V\to\infty$. Namely, it was rigorously proved that a correct vacuum state must have the ''cluster property'' [12], and it was shown for BEC systems that $|N,G\rangle$ does not have this property, whereas the CSIB does [5,7]. This fact and the robustness of the CSIB against weak perturbations from environments [6] strongly suggest that for a sufficiently large V the CSIB should be realized.
[16] See, e.g., R.J. Rivers, *Path Integral Methods in Quantum Field Theory* (Cambridge University Press, Cambridge, 1987), sec. 13.6.
[17] Similar results were previously obtained in Ref. [8], which assumed almost-free bosons and $M=1$. The present result is the generalization to general interacting many-boson systems and to general observables, for which $M \geqslant 1$.