Finite-size scaling behavior of Bose-Einstein condensation in the 1D Bose gas

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Through exact numerical solutions we show Bose-Einstein condensation (BEC) for the one-dimensional (1D) bosons with repulsive short-range interactions at zero temperature by taking a particular large size limit. Following the Penrose-Onsager criterion of BEC, we define condensate fraction by the fraction of the largest eigenvalue of the one-particle reduced density matrix. We show that the finite-size scaling behavior such that condensate fraction is given by a scaling function of one-variable: interaction parameter multiplied by a power of particle number. Condensate fraction is nonzero and constant for any large value of particle number or system size, if the interaction parameter is proportional to the negative power of particle number. Here the interaction parameter is defined by the coupling constant of the delta-function potentials divided by the density. With the scaling behavior we derive various thermodynamic limits where condensate fraction is constant for any large system size; for instance, it is the case even in the system of a finite particle number.

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The experimental realization of trapped atomic gases in one dimension has provided a new motivation for the study of strong correlations in fundamental quantum mechanical systems of interacting particles \[4\]. In one-dimensional (1D) systems quantum fluctuations play a key role and often give subtle and nontrivial effects. It is known that Bose-Einstein condensation (BEC) occurs even for bosons with repulsive interactions due to the quantum statistical effect among identical particles \[4\]. In fact, it has been proven rigorously for interacting bosons confined in dimensions greater than one \[4\]. In 1D case there is no BEC for bosons with repulsive interactions due to strong quantum fluctuations if we take the standard thermodynamic limit with fixed coupling constant \[4\]. On the other hand, if the coupling constant is very weak, we may expect that even the 1D bosons with a large but finite number of particles undergo a quasi-condensation in which “a macroscopic number of particles occupy a single one-particle state” \[4\]. However, it has not been shown explicitly how such a quasi-condensation occurs in interacting bosons in one dimension. Furthermore, it is nontrivial to expect it for the 1D Bose gas that is solvable by the Bethe ansatz. No pair of particles can have the same quasi-momentum in common for a Bethe-ansatz solution. Here we call the 1D system of bosons interacting with repulsive delta-function potentials the 1D Bose gas. For the impenetrable 1D Bose gas where the coupling constant is taken to infinity, condensate fractions are analytically and numerically studied \[7\], while in the weak coupling case it is nontrivial to evaluate the fractions in the 1D Bose gas.

In the present Letter we show the finite-size scaling behavior of condensate fraction in the 1D Bose gas with repulsive interactions at zero temperature, and derive BEC by controlling the thermodynamic limit. We show that if the coupling constant decreases as a power of the system size, condensate fraction does not vanish and remains constant when we send the system size to infinity or to a very large value with fixed density. If condensate fraction is nonzero for a large number of particles, we call it BEC according to the Penrose-Onsager criterion.

The scaling behavior of BEC in the 1D Bose gas is fundamental when we specify the thermodynamic limit, where we send particle number \(N\) or system size \(L\) to infinity or very large values. We define interaction parameter \(\gamma\) by \(\gamma = c/n\) with coupling constant \(c\) in the delta-function potentials and density \(n = N/L\). We show that if \(\gamma\) is given by a negative power of \(N\), i.e., \(\gamma = A/N^\eta\), condensate fraction \(n_0\) is nonzero and constant for any large value of \(L\) or \(N\). We also show that exponent \(\eta\) and amplitude \(A\) are independent of density \(n\), and evaluate them as functions of \(n_0\). Condensate fraction \(n_0\) is thus given by a scaling function of variable \(\gamma N^\eta\). If the condensate fraction of a quantum state with large \(N\) is nonzero in the 1D Bose gas, we suggest that the classical mean-field approximation such as the Gross-Pitaevskii (GP) equation is valid for the state \[8\]. Furthermore, we show that the 1D Bose gas of a finite particle number may have the same condensate fraction for any large \(L\).

Let us review the definition of BEC through the one-particle reduced density matrix for a quantum system \[1, 8\]. We assume that the number of particles \(N\) is very large but finite. At zero temperature, the density matrix is given by \(\hat{\rho} = |\lambda\rangle\langle\lambda|\), where \(|\lambda\rangle\) denotes the ground state of the quantum system. We define the one-particle reduced density matrix by the partial trace of the density matrix with respect to other degrees of freedom: \(\hat{\rho}_1 = N \text{tr}_{23\ldots N} \hat{\rho}\). This matrix is positive definite and hence it is diagonalized as

\[
\hat{\rho}_1 = N_0|\Psi_0\rangle\langle\Psi_0| + N_1|\Psi_1\rangle\langle\Psi_1| + \cdots . \tag{1}
\]

Here we put eigenvalues \(N_j\) in descending order: \(N_0 \geq N_1 \geq N_2 \geq \cdots > 0\). The sum of all the eigenvalues is given by the number of particles: \(\sum_j N_j = N\). Here we
recall $\text{tr}_1 \hat{\rho}_1 = N$ due to the normalization: $\text{tr}_{123\ldots N} \hat{\rho} = 1$. Let us denote by $n_0$ the ratio of the largest eigenvalue $N_0$ to particle number $N$:

$$n_0 := N_0/N.$$  \hspace{1cm} (2)

The criterion of BEC due to Penrose and Onsager \[4\] is given as follows: If the largest eigenvalue $N_0$ is of order $N$, i.e. the ratio $n_0$ is nonzero and finite for large $N$, then we say that the system exhibits BEC, and we call $n_0$ the condensate fraction. Here we also define fractions $n_j$ by $n_j = N_j/N$ for $j = 1, 2, \ldots$. 

We now consider the Hamiltonian of the 1D Bose gas, which we call the Lieb-Liniger model (LL model) \[10\]:

$$\mathcal{H}_{LL} = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2\rho \sum_{j<k} \delta(x_j - x_k).$$  \hspace{1cm} (3)

We assume the periodic boundary conditions of the system size $L$ on the wavefunctions. We employ a system of units with $2m = \hbar = 1$, where $m$ is the mass of the particle. We consider the repulsive interaction: $c > 0$, hereafter.

In the thermodynamic limit the LL model is characterized by the single parameter $\gamma = c/n$, where $n = N/L$ is the density of particle number $N$. We fix the particle-number density as $n = 1$ throughout the Letter, and change coupling constant $c$ so that we have different values of $\gamma$.

In the LL model, the Bethe ansatz offers an exact eigenstate with an exact energy eigenvalue for a given set of quasi-momenta $k_1, k_2, \ldots, k_N$ satisfying the Bethe ansatz equations (BAE) for $j = 1, 2, \ldots, N$:

$$k_j L = 2\pi I_j - 2 \sum_{\ell \neq j}^{N} \arctan \left( \frac{k_j - k_\ell}{c} \right).$$  \hspace{1cm} (4)

Here $I_j$‘s are integers for odd $N$ and half-odd integers for even $N$. We call them the Bethe quantum numbers. The total momentum $P$ and energy eigenvalue $E$ are written in terms of the quasi-momenta as

$$P = \sum_{j=1}^{N} k_j = 2\pi \sum_{j=1}^{N} I_j, \quad E = \sum_{j=1}^{N} k_j^2.$$  \hspace{1cm} (5)

If we specify a set of Bethe quantum numbers $I_1 < \cdots < I_N$, BAE \[4\] have a unique real solution $k_1 < \cdots < k_N$ \[11\]. In particular, the sequence of the Bethe quantum numbers of the ground state is given by $I_j = -(N + 1)/2 + j$ for integers $j$ with $1 \leq j \leq N$. The Bethe quantum numbers for low lying excitations are systematically derived by putting holes or particles in the perfectly regular ground-state sequence.

The matrix element of the one-particle reduced density matrix, $\rho_1(x, y) := \langle x|\hat{\rho}_1|y \rangle$, for a quantum system is expressed as a correlation function in the ground state $|\lambda\rangle$:

$$\rho_1(x, y) = \langle \lambda|\hat{\psi}^\dagger(y)\hat{\psi}(x)|\lambda \rangle.$$  \hspace{1cm} (6)

In the LL model we can numerically evaluate the correlation function by the form factor expansion. Inserting the complete system of eigenstates, $\sum_{\mu} |\mu\rangle\langle\mu|$, we have

$$\rho_1(x, y) = \sum_{\mu} e^{i(P_\mu - P_\lambda)(y - x)} \langle \mu|\hat{\psi}(0)|\lambda \rangle^2,$$  \hspace{1cm} (7)

where $P_\mu$ denote the momentum eigenvalues of eigenstates $|\mu\rangle$. Each form factor in the sum \[7\] is expressed as a product of determinants by making use of the determinant formula for the norms of Bethe eigenstates \[12\] and that for the form factors of the field operator \[13–15\]:

$$\langle \mu|\hat{\psi}(0)|\lambda \rangle = (-1)^{N(N + 1)/2 + 1} \times \left( \prod_{j=1}^{N-1} \prod_{\ell=1}^{N} \frac{1}{k_j^\prime - k_\ell^\prime} \right) \left( \prod_{j > \ell}^{N} k_{j,\ell}^\prime \sqrt{k_{j,\ell}^2 + c^2} \right) \left( \det U(k, k') / \det G(k) \right),$$  \hspace{1cm} (8)

where the quasi-momenta \{k_1, \cdots, k_N\} and \{k'_1, \cdots, k'_{N-1}\} give the eigenstates $|\lambda\rangle$ and $|\mu\rangle$, respectively. Here we have employed the abbreviated symbols $k_{j,\ell} := k_j - k_\ell$ and $k'_j, k'_\ell := k'_j - k'_\ell$. The matrix $G(k)$ is the Gaudin matrix, whose $(j, \ell)$th element is $G(k_{j,\ell}) = \delta_{j,\ell} L + \sum_{m=1}^{N} K(k_{j,m}) - K(k_{\ell,j})$ for $j, \ell = 1, 2, \ldots, N$, where the kernel $K(k)$ is defined by $K(k) = 2c/|k^2 + c^2|$. The matrix elements of the $(N - 1)$ by $(N - 1)$ matrix $U(k, k')$ are given by \[12\] \[13\]:

$$U(k, k')_{j,\ell} = 2\delta_{j,\ell} \text{Im} \left[ \frac{1}{\prod_{\alpha=1}^{N-1} (k_{\alpha} - k_j + ic)} \prod_{\alpha=1}^{N-1} (k_{\alpha} - k_j - ic) \right] + \prod_{\alpha \neq j}^{N} \frac{1}{(k_{\alpha} - k_j)} \left( K(k_{j,\ell}) - K(k_{\ell,j}) \right).$$  \hspace{1cm} (9)

Numerically we calculate correlation function \[14\] by taking the sum over a large number of eigenstates with

| $c$ | 0.01 | 1 | 100 |
|-----|------|---|-----|
| 1p1h | 0.999984 | 0.971538 | 0.693620 |
| 2p2h | 1.59454 x 10^{-5} | 0.0280102 | 0.289056 |
| $n_{sat}$ | 1.00000 | 0.999548 | 0.982676 |

TABLE I: Fraction $n_{sat}$ of the reduced density operator at the origin, $\rho_1(0, 0)$, to the density $n$, evaluated by taking the sum over a large number of eigenstates $|\mu\rangle$ with one particle and one hole (1p1h) or with two particles and two holes (2p2h) for $N = L = 50$ ($n = 1$): $n_{sat} = \left( \sum_{\mu \text{1p1h}} + \sum_{\mu \text{2p2h}} \right) \langle |\mu|\hat{\psi}(0)|\lambda \rangle^2 / n.$
FIG. 1: (Color online) Dependence of fractions $n_j$ on coupling constant $c$. In the upper panel: condensate fraction $n_0$ is plotted against coupling constant $c$ for $N = 4$, 10, 20, 40, 100, 200, and 400, from the top to the bottom, in red, green, blue, black, orange, purple, and cyan lines, respectively. In the lower panel: condensate fraction $n_0$, fractions $n_1$ and $n_2$ are shown against $c$ from the top to the bottom in blue, red and green lines, respectively, for $N = 20$. We recall $n = N/L = 1$.

The eigenvalues of the one-particle reduced density matrix are given by plane waves $\hat{\rho}_0$ (0,0)/$n$, through the form factor expansion (7) for the excitations with 1p1h or 2p2h. We denote it by $n_{\text{sat}}$. The estimates of $n_{\text{sat}}$ are listed in Table 1. The graph of $n_{\text{sat}}$ approaches 1 for small coupling constant $c$, while it is larger than 0.98 for any value of $c$ in the case of $N = 50$.

For the LL model, the eigenfunctions of the one-particle reduced density matrix are given by plane waves for any nonzero and finite value of $c$. It is a consequence of the translational invariance of the Hamiltonian of the LL model. We thus have

$$\rho_1(x, y) = \frac{N_0}{L} + \sum_{j=1}^{\infty} \frac{2N_j}{L} \cos[2\pi j(x - y)/L].$$  (10)

The eigenvalues of the one-particle reduced density matrix, $N_j$, are expressed in terms of the form factor expansion. We consider the sum over all the form factors between the ground state, $|\lambda\rangle$, and such eigenstates, $|\mu\rangle$, that have a given momentum $P_j$ as

$$N_j = L \sum_{\mu: P_\mu = P_j} |\langle \mu | \hat{\psi}(0) | \lambda \rangle|^2.$$  (11)

FIG. 2: (Color online) Condensate fraction $n_0$ as a function of $1/N$ for $c = 0.01$. Here $N = N/L = 1$.

In the LL model we have $P_j := (2\pi/L)j$.

Solving the Bethe ansatz equations for a large number of eigenstates we observe numerically that eigenvalues $N_j$ are given in decreasing order with respect to integer $j$: $N_0 > N_1 > N_2 > \cdots$. It thus follows that condensate fraction which corresponds to the largest eigenvalue of the one-particle reduced density matrix $\hat{\rho}_0$ is indeed given by $n_0 = N_0/N$, where $N_0$ has been defined by sum (11) over all eigenstates with zero momentum.

The estimates of condensate fraction $n_0$ are plotted against coupling constant $c$ in the upper panel of Fig. 1 over a wide range of $c$ such as from $c = 10^{-3}$ to $c = 10^3$ for different values of particle number $N$ such as $N = 4$, 10, 20, 400. For each $N$, condensate fraction $n_0$ becomes 1.0 for small $c$ such as $c < 0.01$, while it decreases with respect to $c$ and approaches an asymptotic value in the large $c$ region such as $c > 100$ or 1000. The asymptotic values depend on particle number $N$ for $N = 4$, 10, 20, 400, and they are consistent with the numerical estimates of occupation numbers for the impenetrable 1D Bose gas (see eq. (56) of Ref. 7). In the lower panel of Fig. 1 we plot fractions $n_j$ for $j = 0, 1$ and 2 against coupling constant $c$ from $c = 10^{-3}$ to $c = 10^3$ with $N = 40$. The asymptotic values of $n_j$ for large $c$ (i.e. $c = 1000$) are consistent with the numerical estimates for the impenetrable 1D Bose gas (for $n_1$ and $n_2$, see eqs. (57) and (58) of Ref. 7, respectively).

We observe that condensate fraction $n_0$ decreases as particle number $N$ increases when density $n = N/L$ is fixed. It is the case for $c < 0.1$ in the upper panel of Fig. 1. Condensate fraction $n_0$ decreases as $N$ increases even for small $c$ such as $c = 0.01$, as shown in Fig. 2. Thus, it is necessary for coupling constant $c$ to decrease with respect to $N$ so that condensate fraction $n_0$ remains constant as $N$ increases with fixed density $n$.

We now show the finite-size scaling of condensate frac-
tion $n_0$. In Fig. 3 each contour line gives the graph of interaction parameter $\gamma$ as a function of the inverse of particle number $N$ for a fixed value of condensate fraction $n_0$. They are plotted for various values of $n_0$ from $n_0 = 0.6$ to 0.99, and are obtained by solving the Bethe-ansatz equations numerically. For different values of density such as $n = 1, 2$ and 5, we plot contour lines with fixed values of condensate fraction $n_0$ in the plane of interaction parameter $\gamma$ versus inverse particle number $1/N$. We observe that the contours with the same condensate fraction $n_0$ for the different densities coincide in the $\gamma$ versus $1/N$ plane and are well approximated by

$$\gamma = A/N^\eta.$$  \hfill (12)

Thus, condensate fraction $n_0$ is constant as particle number $N$ becomes very large if interaction parameter $\gamma$ is given by the power of particle number $N$ as in eq. (12).

Applying the finite-size scaling arguments, we suggest from eq. (12) that condensation fraction $n_0$ is given by a scaling function $\phi(\cdot)$ of a single variable $\gamma N^n$: $n_0 = \phi(\gamma N^n)$. Here we recall the coincidence of contours for the different values of density $n$ in Fig. 3. We thus observe that exponent $\eta$ and amplitude $A$ of eq. (12) are determined only by condensate fraction $n_0$ and are independent of density $n$.

Let us consider amplitude $A$ as a function of $n_0$. We denote it by $A = f(n_0)$. Then, the scaling function $\phi(\cdot)$ is given by the inverse function: $n_0 = f^{-1}(A)$. In Fig. 4 exponent $\eta$ increases with respect to $n_0$, and amplitude $A$ decreases monotonically with respect to $n_0$.

It follows from (12) that BEC does not occur in the 1D Bose gas if we fix parameter $\gamma$ and density $n$ as system size $L$ goes to infinity. However, if $\gamma$ is small enough so that it satisfies eq. (12) for a given value of condensate fraction $n_0$, the 1D Bose gas shows BEC from the viewpoint of the Penrose and Onsager criterion. We suggest that if condensate fraction $n_0$ of a quantum state is nonzero and finite for large $N$, the mean-field approximation is valid for the quantum state. For instance, there exist such quantum states that correspond to classical dark solitons of the GP equation [8], if parameter $\gamma$ is small enough so that it satisfies (12).

With the scaling behavior (12) we derive various ways of the thermodynamic limit such that condensate fraction $n_0$ is constant. For instance, we consider the case of a finite particle number, $N = N_L$. Choosing a value of $n_0$, we determine $\gamma$ by eq. (12) as $\gamma = A(n_0)/N_L^{\eta(n_0)}$. Then, the 1D Bose gas with $N = N_L$ has the same condensate fraction $n_0$ for any large value of $L$ if coupling constant $c$ is given by $c = A(n_0) N_L^{1-\eta}/L$. Let us set $\eta = 1$ and $N_L = 10$, for simplicity. We have $n_0 = 0.97$ in Fig. 4 and $\gamma = 0.3$ at $1/N = 0.1$ in the contour of $n_0 = 0.97$ in Fig. 3. By assuming $n = 1$, it corresponds to the case of $L = 10$ and $c = 0.3$, and we have $A = c L = 3$, which is consistent with Fig. 4. Therefore, the 1D Bose gas with $N_L = 10$ has $n_0 = 0.97$ for any large $L$ if $c$ is given by $c = 0.3/L$. Moreover, we may consider other types of thermodynamic limits. When density $n$ is proportional to a power of $L$ as $L^\alpha$, condensate fraction $n_0$ is constant as $L$ goes to infinity if we set $c \propto L^{(1-\eta)(1+\alpha)-1}$.
The scaling law \([12]\) and the estimates of condensate fraction in the present Letter should be useful for estimating conditions in experiments of trapped cold atomic gases in one dimension \([16]\). For instance, we suggest from Fig. 1 that BEC may appear in 1D systems with a small number of bosons such as \(N = 20\) or \(40\) for \(c = 1\) or \(10\).

In conclusion, we exactly calculated the condensate fraction of the 1D Bose gas with repulsive interaction by the form factor expansion. We have shown the finite-size scaling behavior such that condensate fraction \(n_0\) is given by a scaling function of interaction parameter \(\gamma\) times some power of particle number \(N\): \(n_0 = \phi(\gamma N^\eta)\). Consequently, if parameter \(\gamma\) decrease as \(\gamma = A/N^\eta\), condensate fraction \(n_0\) remains nonzero and constant as particle number \(N\) becomes very large. By modifying the thermodynamic limit, the 1D Bose gas shows BEC from the viewpoint of the Penrose-Onsager criterion.

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[1] A. Görlitz, J.M. Vogels, A.E. Leanhardt, C. Raman, T.L. Gustavson, J.R. Abo-Shaeer, A.P. Chikkatur, S. Gupta, S. Inouye, T. Rosenband and W. Ketterle, Phys. Rev. Lett. 87, 130402 (2001).

[2] M. Greiner, I. Bloch, O. Mandel, T.W. Hänsch, and T. Esslinger, Phys. Rev. Lett. 87, 160405 (2001).

[3] T. Kinoshita, T. Wenger and D.S. Weiss, Science 305, 1125 (2004); Phys. Rev. Lett. 95, 190406 (2005); Nature 440, 900 (2006).

[4] A.J. Leggett, Quantum Liquids (Oxford University Press, 2006).

[5] E.H. Lieb and R. Seiringer, Phys. Rev. Lett. 88, 170409 (2002).

[6] L. Pitaevskii and S. Stringari, J. Low Temp. Phys. 85, 377 (1991).

[7] P.J. Forrester, N.E. Frankel, T.M. Garoni, and N.S. Witte, Phys. Rev. A 67, 043607 (2003).

[8] J. Sato, R. Kanamoto, E. Kaminishi, and T. Deguchi, Phys. Rev. Lett. 108, 110401 (2012).

[9] O. Penrose, L. Onsager, Phys. Rev. 104, 576 (1956).

[10] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963); E. H. Lieb, Phys. Rev. 130, 1616 (1963).

[11] V.E. Korepin, N.M. Bogoliubov and A.G. Izergin, Quantum Inverse Scattering Method and Correlation Functions (Cambridge University Press, Cambridge, 1993)

[12] M. Gaudin, “La fonction d onde de Bethe”, Masson (Paris) (1983); V. E. Korepin, Commun. Math. Phys. 86, 391 (1982).

[13] J.-S. Caux, P. Calabrese and N. A. Slavnov, J. Stat. Mech. P01008 (2007).

[14] N. A. Slavnov, Theor. Mat. Fiz. 79, 232 (1989); 82, 389 (1990);

[15] T. Kojima, V.E. Korepin, N.A. Slavnov, Commun. Math. Phys. 188, 657 (1997).

[16] L. Pitaevskii and S. Stringari, Bose-Einstein Condensation (Oxford University Press, 2003).