Critical nature of ideal Bose-Einstein condensation: Similarity with Yang-Lee theory of phase transition

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It is found that the singularity of the thermodynamic potential of an ideal Bose gas is connected with the physical root $z_0=1$ of the inverse of the grand partition function. The critical nature is determined solely by the behavior of the root distribution of the inverse of the grand partition function near $z_0=1$. This is quite similar to the situation of phase transition described by Yang-Lee theory. [S1063-651X(99)12801-0]

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In 1924 Einstein [1] generalized Bose's novel derivation of Planck's blackbody radiation law and proposed the Bose-Einstein statistics. He calculated the thermodynamic properties of an ideal Bose gas and found that below the critical temperature, particles begin to condense in the lowest energy level and the gas undergoes a phase transition, known as Bose-Einstein condensation (BEC). In 1938, London [2] used BEC to explain the superfluidity of liquid helium. Penrose and Onsager [3] proposed a generalized criterion of BEC. Yang [4] further extended this criterion to superfluid and superconductivity and proposed the concept of off-diagonal long-range order. For many years, ideal BEC was regarded as a mathematical artifact. Fortunately, in recent years, nearly ideal BEC have been observed in experiments [5]. These experimental works greatly stimulated theoretical studies.

Ideal BEC was studied in some respects, such as in any dimension [6–9], in critical nature as an ordinary phase transition [10]. A similarity with the spherical model was established [10]. Furthermore, ideal BEC in relativistic ideal Bose gas was studied [11].

In this paper, we shall show that similar to the nature of phase transitions described by Yang-Lee theory, the critical nature of ideal BEC is determined solely by the behavior of the root distribution of the inverse of the grand partition function near the physical root $z_0=1$.

In dimension d, for an ideal Bose gas, the number of particles and the energy of the gas are given, respectively, by

$$N=N(\epsilon=0)+N(\epsilon\neq 0)=N(\epsilon=0)+B(d)\int_0^\infty \frac{1}{e^{(\epsilon-\mu)/T}-1}p^{d-1}dp=N(\epsilon=0)+B(d)\int_0^\infty \frac{1}{e^{(\epsilon-\mu)/T}-1}g(\epsilon)d\epsilon, \qquad (1)$$

$$E(T)=B(d)\int_0^\infty \frac{\epsilon}{e^{(\epsilon-\mu)/T}-1}g(\epsilon)d\epsilon, \qquad (2)$$

where $B(d)=2V\pi^{d/2}/\Gamma(d/2)$ and $g(\epsilon)=p^{d-1}(dp/d\epsilon)$ is the distribution function of quantum states. $N(\epsilon=0)$ and $N(\epsilon\neq 0)$ are the number of particles distributed on the energy levels $\epsilon=0$ and $\epsilon\neq 0$, respectively. Throughout this paper we use the system of units $k_B=h=1$. The chemical potential $\mu\leqslant 0$ is required in order to have the positive definiteness of particle distribution. For $T>T_c$, $\mu<0$ and $N(\epsilon=0)=0$; for $T=T_c$, $\mu=0$ and $N(\epsilon=0)=0$; for $T<T_c$, $\mu=0$ and $N(\epsilon=0)\neq 0$. The critical temperature is defined by

$$N=B(d)\int_0^\infty \frac{1}{e^{\epsilon/T_c}-1}g(\epsilon)d\epsilon. \qquad (3)$$

Assume that near the ground state, the energy spectrum has the property $\epsilon(p)\to ap^\lambda$ as $p\to 0$ (λ is a positive exponent). Thus the quantum state distribution function has the property $g(\epsilon)\to\epsilon^{d/\lambda-1}$ as $\epsilon\to 0$. It is easy to verify that if $d/\lambda>1$, the integrand in Eq. (3) is convergent and T_c is finite. Let $d/\lambda-1=\alpha$. We show that the critical nature of ideal BEC is determined solely by the behavior of the quantum state distribution function near the ground state. The following states this more clearly.

Theorem. For an ideal Bose gas, if the quantum state distribution has the behavior $g(\epsilon)\to\epsilon^\alpha$ as $\epsilon\to 0$ and α is a positive exponent, the gas will undergo a phase transition at finite temperature. In this case, the nature of the phase transition is determined completely by α: 1. If $\alpha>1$, the phase transition is second order, with a finite jump in C_V. 2. If $1/2<\alpha\leqslant 1$, C_V is continuous, with infinite jump in $(\partial C_V/\partial T)_{T_c}$ and $(\partial C_V/\partial T)_{T_c^+}=-\infty$. 3. If $\alpha=1/2$, C_V is continuous, with a finite jump in $(\partial C_V/\partial T)_{T_c}$. 4. If $0<\alpha<1/2$, (a) if $\alpha=1/(n+1)$ $(n=2,3,\ldots)$, $(\partial^{n-1}C_V/\partial T^{n-1})_{T_c}$ is continuous, with a finite jump in $(\partial^n C_V/\partial T^n)_{T_c}$; (b) if $1/(n+2)<\alpha<1/(n+1)$ $(n=1,2,\ldots)$, $(\partial^n C_V/\partial T^n)_{T_c}$ is continuous, with an infinite jump in $(\partial^{n+1}C_V/\partial T^{n+1})_{T_c}$ and $(\partial^{n+1}C_V/\partial T^{n+1})_{T_c^+}=\infty$.

Proof. Define the following functions:

$$N_0(T)=B(d)\int_0^\infty \frac{1}{e^{\epsilon/T}-1}g(\epsilon)d\epsilon, \qquad (4)$$

$$E_0(T)=B(d)\int_0^\infty \frac{\epsilon}{e^{\epsilon/T}-1}g(\epsilon)d\epsilon. \qquad (5)$$

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Their physical meanings are that for $T<T_c$, $N_0(T)=N(\epsilon\neq 0)$ and $E_0(T)=E(T)$. Consider $T>T_c$:

$$
\begin{aligned}
N_0(T)-N&=B(d)\int_0^\infty\left[\frac{1}{e^{\epsilon/T}-1}-\frac{1}{e^{(\epsilon-\mu)/T}-1}\right]g(\epsilon)d\epsilon\\
&=B(d)(e^{-\mu/T}-1)\\
&\quad\times\int_0^\infty\frac{e^{\epsilon/T}}{[e^{(\epsilon-\mu)/T}-1](e^{\epsilon/T}-1)}g(\epsilon)d\epsilon\\
&\equiv B(d)(e^{-\mu/T}-1)I_1(\mu,T).
\end{aligned}\tag{6}
$$

Let us split up the integrand $I_1(\mu,T)$ into two parts. The first part ($I_1^{(1)}$) is integrated from 0 to ϵ_0. We choose ϵ_0 and μ such that $g(\epsilon)=(\lambda a^{d/\lambda})^{-1}\epsilon^\alpha$ for $\epsilon\leqslant\epsilon_0$ and $-\mu\ll\epsilon_0\ll T$. Thus for $0<\alpha<1$,

$$
\begin{aligned}
I_1^{(1)}&=b\int_0^{\epsilon_0}\frac{1}{(\epsilon-\mu)\epsilon}\epsilon^\alpha d\epsilon\\
&=b|\mu|^{\alpha-1}\int_0^\infty\frac{x^{\alpha-1}}{1+x}dx\\
&=[b\pi/\sin(\alpha\pi)]|\mu|^{\alpha-1},
\end{aligned}\tag{7}
$$

where $b=T^2a^{-d/\lambda}\lambda^{-1}$, $x=\epsilon/|\mu|$ and we take the integration upper limit $\epsilon_0/|\mu|$ as infinity. For $\alpha=1$,

$$
I_1^{(1)}=b\int_0^{\epsilon_0}\frac{1}{\epsilon-\mu}d\epsilon=b(\ln\epsilon_0-\ln|\mu|)\tag{8}
$$

For $\alpha>1$, $I_1(\mu\to 0,T)$ is convergent. Thus

$$
I_1(\mu\to 0,T)\to\begin{cases} I_1(0,T), & \alpha>1,\\ -b\ \ln(-\mu), & \alpha=1,\\ b_1(-\mu)^{\alpha-1}, & 0<\alpha<1,\end{cases}\tag{9}
$$

where $b_1=b\pi/\sin(\alpha\pi)$. On the other hand, using Eq. (3), we find that as $T\to T_c^+$,

$$
\begin{aligned}
N_0(T)-N&=B(d)\int_0^\infty\left(\frac{1}{e^{\epsilon/T}-1}-\frac{1}{e^{\epsilon/T_c}-1}\right)g(\epsilon)d\epsilon\\
&\approx B(d)\left(\frac{1}{T_c}-\frac{1}{T}\right)\int_0^\infty\frac{\epsilon e^{\epsilon/T}}{(e^{\epsilon/T_c}-1)(e^{\epsilon/T}-1)}g(\epsilon)d\epsilon\\
&\equiv[B(d)I_2(T)/T]t,
\end{aligned}\tag{10}
$$

where $t=(T-T_c)/T_c$. It is easy to show that $I_2(T)$ is convergent and analytic if $\alpha>0$. Therefore identifying Eq. (6) with (10) and using Eq. (9), we obtain, in the limit $T\to T_c^+$,

$$
-\mu=\begin{cases}[I_2(T)/I_1(0,T)]\ t, & \alpha>1,\\ -[I_2(T)/b]t[\ln(-\mu)]^{-1}, & \alpha=1,\\ b_2t^{1/\alpha}, & 0<\alpha<1,\end{cases}\tag{11}
$$

where $b_2=[I_2(T)\sin(\alpha\pi)/\pi b]^{1/\alpha}$. Since as $T\to T_c^+$,

$$
\begin{aligned}
E_0(T)-E(T)&=B(d)\int_0^\infty\left(\frac{1}{e^{\epsilon/T}-1}-\frac{1}{e^{(\epsilon-\mu)/T}-1}\right)\epsilon g(\epsilon)d\epsilon\\
&=B(d)(e^{-\mu/T}-1)\\
&\quad\times\int_0^\infty\frac{\epsilon e^{\epsilon/T}}{[e^{(\epsilon-\mu)/T}-1](e^{\epsilon/T}-1)}g(\epsilon)d\epsilon\\
&\equiv B(d)(e^{-\mu/T}-1)I_3(\mu,T)\\
&\approx B(d)I_3(0,T)(-\mu/T),\quad\text{as }\ \mu\to 0
\end{aligned}\tag{12}
$$

where the integrand $I_3(0,T)$ is convergent and analytic. Substituting Eq. (11) into Eq. (12) yields

$$
E(T)=\begin{cases}E_0(T)-f_1(T)t, & \alpha>1,\\ E_0(T)+f_2(T)t[\ln(-\mu)]^{-1}, & \alpha=1,\\ E_0(T)-f_3(T)t^{1/\alpha}, & 0<\alpha<1,\end{cases}\tag{13}
$$

where $f_1(T)=B(d)I_2(T)I_3(0,T)/TI_1(0,T)$, $f_2(T)=B(d)I_2(T)I_3(0,T)/Tb$, and $f_3(T)=B(d)I_3(0,T)b_2/T$. Since $C_V=[\partial E(T)/\partial T]$, as $T\to T_c^+$,

$$
C_V(T)=\begin{cases}\dfrac{\partial E_0(T)}{\partial T}+\text{const}, & \alpha>1,\\[2mm] \dfrac{\partial E_0(T)}{\partial T}+\text{const}\times[\ln(-\mu)]^{-1}, & \alpha=1,\\[2mm] \dfrac{\partial E_0(T)}{\partial T}+\text{const}\times t^{-1+1/\alpha}, & 0<\alpha<1.\end{cases}\tag{14}
$$

Since for $T<T_c$, $E(T)=E_0(T)$, it is easy to find the difference of $\partial C_V/\partial T$ or higher order derivatives on both sides of the critical point. For $\alpha=1$, although C_V is continuous at T_c, $(\partial C_V/\partial T)_{T_c}$ is not continuous,

$$
\left(\frac{\partial C_V}{\partial T}\right)_{T_c^+}=\left[\frac{\partial^2E_0(T)}{\partial T^2}\right]_{T_c}+\text{const}\times[\mu(\ln(-\mu))^3]^{-1}\to\infty.\tag{15}
$$

For $0<\alpha<1/2$, (a) if $\alpha=1/(n+1)$ $(n=2,3,\dots)$, thus as $T\to T_c^+$,

$$
C_V(T)=\frac{\partial E_0(T)}{\partial T}+\text{const}\times t^n.\tag{16}
$$

(b) If $1/(n+2)<\alpha<1/(n+1)$ $(n=1,2,\dots)$, thus as $T\to T_c^+$,

$$
C_V(T)=\frac{\partial E_0(T)}{\partial T}+\text{const}\times t^\tau\quad(n<\tau<n+1).\tag{17}
$$

This completes the proof.

This theorem generalizes the result derived by de Groot, Hooyman, and ten Seldam [6].

In 1952 Yang and Lee [12] proposed a phase transition theory. They observed that for a real interacting gas, the pair interaction has hard core. For a given volume V, the maximum number M of particles that can be crammed into the volume is limited by the size of the hard core, i.e., M

$\sim V/a^3$. Here a is the radius of the hard core. Thus the grand partition function can be expressed as a polynomial of fugacity $z=\exp(\mu/T)$,

$$\Xi=\sum_{n=0}^{M} z^n Q_n/n! = \prod_{l=1}^{M}\left(1-\frac{z}{z_l}\right), \tag{18}$$

where $Q_n>0$ is the partition function of the system with n particles in the volume V. The roots z_l are never positive real. The root distribution can touch the positive real axis only in the thermodynamic limit and give the transition point. The singularity of the thermodynamic potential is connected with the positive real root. They took the lattice gas model as an example and found that the nature of the phase transition is determined solely by the behavior of the root distribution near the positive real root. In this example the roots are located on an unit circle in the complex $y=\exp\{\mu-(1/2)\phi]/T\}$ plane (Yang-Lee circle theorem), namely, $y_l=\exp(i\theta_l)$ [13]. Here $\phi=\Sigma_{j(\neq i)}u(r_{ij})$ is the potential energy among any atom i and other atoms and $u(r_{ij})<0$ the attractive pair potential energy. Thus the pressure is given by

$$P=\frac{T}{V}\ln\Xi=\frac{T}{V}\sum_l \ln\left(1-\frac{y}{y_l}\right)$$
$$=T\int_0^{\pi} g(\theta)\ln(y^2-2y\cos\theta+1)d\theta, \tag{19}$$

where $g(\theta)$ is the root distribution function. $\theta=0$ corresponds to the positive real root $y_l=1$. When $\theta\to 0$, if $g(\theta)\to g(0)+b|\theta|^{\nu}+\cdots$ $(\nu>0)$, Yang and Lee showed that the $g(0)$ term gives a flat horizontal portion on the P-V diagram. Let $m-1<n\leq m$ (m is a positive integer). The next term gives a jump in the mth derivative of V with respect to P.

In 1964 Fisher [14] observed that for some kinds of lattice models, the partition function can be expressed as a polynomial. He discussed the roots of the partition function in the complex temperature plane. He used the square lattice Ising model as an example and also found that the critical nature is determined solely by the behavior of root distribution near the positive real root. In this example the roots are located on an unit circle in the complex $x=\sinh 2J/T$ plane, namely, $x_l=\exp(i\theta_l)$. Then the free energy is

$$f=T\sum_l \ln\left(1-\frac{x}{x_l}\right)=\int_0^{\pi} g(\theta)\ln(x^2-2x\cos\theta+1)d\theta. \tag{20}$$

Fisher proved that the root distribution $g(\theta)\to|\theta|$ near $\theta=0$ gives the logarithmic singularity of the two-dimensional Ising model. For the q-state Potts model [15,16], it was found that in the complex $x=(e^{J/T}-1)/\sqrt{q}$ plane, the roots in the Re $x>0$ region are located on the unit circle $|x|=1$. As $\theta\to 0$, $g(\theta)\to|\theta|^{1-\alpha(q)}$ for $q\leq 4$, which gives the specific heat singularity $|t|^{-\alpha(q)}$ (second-order phase transition); and $g(\theta)\to f(q)$ for $q>4$, which gives a first order phase transition with latent heat $f(q)$.

For an ideal Bose gas, since no hard core exists, the grand partition function is an infinite power series of fugacity and can not be expressed as a polynomial of fugacity. So we can not introduce the roots of the grand partition function. Nevertheless, the inverse of the grand partition function can be expressed as

$$\Xi^{-1}=\prod_k\left(1-\frac{z}{\exp(\epsilon_k/T)}\right), \tag{21}$$

where the product is taken over each quantum state k. Similar to the Yang-Lee approach, we can introduce the roots of Ξ^{-1},

$$z_k=\exp(\epsilon_k/T). \tag{22}$$

It is seen that the root distribution is determined by the energy spectrum. Since

$$-\ln\Xi=\sum_k \ln\left(1-\frac{z}{\exp(\epsilon_k/T)}\right)$$
$$\to B(d)\int_0^{\infty} g(\epsilon)\ln\left(1-\frac{z}{\exp(\epsilon/T)}\right)d\epsilon, \tag{23}$$

we identify the root distribution function with the quantum state distribution function $g(\epsilon)=p^{d-1}(dp/d\epsilon)$.

Since physically $\mu\leq 0$ and $\epsilon_k\geq 0$, so $z\leq 1$ and $z_k\geq 1$. When $\mu=0$, $\epsilon_k=0$, we have the unique physical root $z=z_0=1$, which corresponds to the singularity of the grand partition function ($\Xi=\infty$) and the thermodynamic potential. From theorem 1 we know that if $g(\epsilon)\to\epsilon^{\alpha}$ as $\epsilon\to 0$, then the critical nature of ideal BEC is determined completely by α. Therefore the critical nature of ideal BEC is determined solely by the root distribution near $z_0=1$, namely, $g(\epsilon\to 0)\to\epsilon^{\alpha}$. We obtain the following conclusion.

For an ideal Bose gas, the roots of the inverse of the grand partition function are given by $z_k=\exp(\epsilon_k/T)$. The singularity of thermodynamic potential is connected with the physical root $z_0=z=1$. If the root distribution function has the behavior $g(\epsilon)\to\epsilon^{\alpha}$ (α is a positive exponent) as $\epsilon\to 0$, then the critical nature is determined completely by α. In other words, the critical nature of ideal BEC is determined solely by the behavior of the root distribution near the physical root $z_0=1$.

The situation is quite similar to that of phase transitions described by Yang-Lee theory. It is interesting to note that this physical root $z_0=1$ can occur in a finite system, while the positive real root in the Yang-Lee approach occurs in the thermodynamic limit.

We further discuss the difference between ideal BEC and nonideal BEC. The origin of singularity of thermodynamic potential of an ideal Bose gas is quite different from that of a real interacting Bose gas. For a real interacting Bose gas, the pair interaction has a hard core and Yang-Lee theory is applicable. The singularity of the thermodynamic potential is connected with the positive real root of the grand partition function. On the contrary, for ideal Bose gas, the singularity of the thermodynamic potential is connected with the physical root $z_0=z=1$ of the inverse of the grand partition function.

From the above, we further see the following: (1) Ideal BEC can occur in a finite system [17]. This explains why a nearly ideal Bose atom cluster in some experiments [5,18], only with number of particles, say 10^5, that is far from reaching the thermodynamic limit, still has ideal BEC. While for a real interacting Bose gas, nonideal BEC can occur only in the thermodynamic limit; (2) Both singularities of thermodynamic potentials of a real interacting Bose gas and a real interacting classical gas are connected with the positive real roots of their grand partition functions, respectively. Therefore this explains why BEC of a real interacting Bose gas more closely resembles an ordinary gas-liquid phase transition than the ideal BEC, as noted long ago by Huang, Yang, and Luttinger [19,20].

In conclusion, we have found that the singularity of thermodynamic potential of an ideal Bose gas is connected with the physical root $z_0 = z = 1$ of the inverse of the grand partition function. The critical nature of ideal Bose-Einstein condensation is determined solely by the behavior of the root distribution of the inverse of the grand partition function near the physical root $z_0 = 1$. The situation is quite similar to that of phase transition described by Yang-Lee theory, where the nature of the phase transition is determined solely by the behavior of the root distribution of the grand partition function near the positive real root.

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