

Bose-Einstein Condensation of Small Systems

Ruitian Lang, Vladimir Rosenhaus*

MIT Department of Physics

(Dated: May 14, 2008)

We look at the Yang-Lee zeros in the complex temperature plane of Bose-Einstein condensate in a harmonic trap of dimensions 2 – 5. We apply the Grossmann classification scheme to characterize the phase transition. We observe how the true phase transition is approached in the infinite particle number limit. We find the scaling with respect to particle number of the imaginary part of the zero of the canonical partition function closest to the real axis.

1. INTRODUCTION

¹ In 1952 Yang and Lee [1] proposed studying phase transitions by looking at the distribution of zeros in the complex temperature plane of the grand partition function. Yang and Lee showed that the grand partition function can be written as a function of its zeros and for systems with hard-core interactions, the zeros lie on a unit circle. Grossmann *et al.* [2] extended this approach to look at the zeros in the complex temperature plane of the canonical partition function (Z). Since then, the method of studying the zeros of the partition function has been applied to a number of lattice models and systems.

For a finite number of particles, the partition function is obviously analytic. The singularities in various thermodynamic functions arise only in the limit as the number of particles goes to infinity. The power of the method introduced by Yang and Lee is that it gives a way of seeing how this limit is approached. Since phase transition only occur in the limit of an infinite number of particles, for a finite number of particles the zeros can not lie on the real axis. As the infinite particle number limit is approached, the zeros approach the real axis. The phase transition then occurs at the limiting point. The main question when studying small systems is how can the phase transitions observed in small systems be related to the true phase transitions in infinite systems.

One of the most well known phase transitions occurs in Bose-Einstein condensate. Bose-Einstein condensate was successfully produced through confinement in a magnetic field [3] and later through confinement in an optical dipole trap [4]. In these experiments the number of particles in the traps is finite and fixed. However, the standard textbook description of Bose-Einstein condensation is done through the grand canonical ensemble of a noninteracting gas. Therefore, it is useful to have a description of Bose-Einstein condensate for a fixed number of particles. For this purpose [5] introduce a fourth type

of statistical ensemble, which they call Maxwell's demon ensemble, where only particle transfer (without energy exchange) is allowed.

Grossmann *et al.* came up with a classification scheme by which two parameters completely classify the phase transition. Borrmann *et al.* [6], [7], [8] extended this scheme by introducing a third parameter τ_1 which is the imaginary part of the zero of Z closest to the real axis. Borrmann *et al.* found the three classification parameters for Bose-Einstein condensate in a three-dimensional harmonic trap.

In this paper we expand on the work of [7] and look at the zeros of the Z for a Bose-Einstein condensate in a trap of dimension varying from 2 to 5 for a fixed particle number. We concentrate on the parameter τ_1 which is unique to small systems and find its scaling exponent (ρ) with respect to the number of particles in the trap (N). We find that ρ is fairly independent of dimension and we attempt to give a Renormalization Group explanation of ρ .

The paper is organized as follows: in section 2 we give a derivation of the recurrence relations needed to find Z for bosons (this was derived in [6], but our derivation is somewhat different). In section 3 we discuss the nature of the zeros of Z . In section 4 we present the classification scheme of parameters. In section 5 we give our results for the classification parameters. Finally, in section 6 we present an outline of a renormalization group scheme by which to find the exponent ρ .

2. GENERATING FUNCTIONS AND RECURRENCE RELATIONS

We begin by deriving a generating function for the canonical partition function of a degenerate Bose (Fermi) gas. We assume that the eigenstates of the Hamiltonian are labeled by i and the i^{th} eigenstate has energy ϵ_i . The grand partition function $\Xi(\beta)$ is related to the canonical partition function by

$$\Xi(\beta, x) = \sum_{N=0}^{\infty} Z_N(\beta) x^{-N}, \quad (1)$$

where x is the reciprocal of the fugacity and $Z_N(\beta)$ is the partition function for a system with N particles. For

*Electronic address: percyl@mit.edu, vladr@mit.edu

¹ RL wrote the code to find the zeros in C, VR wrote the code in mathematica, and the results agreed. RL provided the derivation of the RG method to find ρ and provided the table of τ_1 . VR provided the steps for the derivation of the recurrence relations for Z and η_0 , and prepared the graph of η_0 .

sufficiently large x , the series converges uniformly, so we have

$$Z_N(\beta) = \frac{1}{2\pi i} \int_C \Xi(\beta, x) x^{N-1} dx, \quad (2)$$

where C is a circle around the origin with sufficiently large radius. For the convenience of later development, we write $\Xi(\beta, x)$ as

$$\begin{aligned} \Xi(\beta, x) &= \prod_i \sum_k \exp(-k\beta\epsilon_i) x^{-k} \\ &= \exp\left(\sum_i \mp \ln(1 \mp \exp(-\beta\epsilon_i)x^{-1})\right) \\ &= \exp\left(\sum_i \sum_{k=1}^{\infty} (\pm 1)^{(k-1)} \exp(-k\beta\epsilon_i) x^{-k}/k\right) \\ &= \exp\left(\sum_{k=1}^{\infty} (\pm 1)^{k-1} \frac{Q_k(\beta)}{k} x^{-k}\right), \end{aligned}$$

where $Q_k = \sum_i \exp(-k\beta\epsilon_i)$ and “+” corresponds to boson systems and “-” corresponds to fermion systems. We substitute the above into (2) to obtain the final form of the generating function

$$Z_N(\beta) = \frac{1}{2\pi i} \int_C \exp\left(\sum_{k=1}^{\infty} (\pm 1)^{k-1} \frac{Q_k(\beta)}{k} x^{-k}\right) x^{N-1} dx \quad (3)$$

By the Cauchy integral formula, this can be recast as

$$Z_N(\beta) = \frac{1}{N!} \frac{d^N}{dx^N} \exp\left(\sum_{k=1}^{\infty} (\pm 1)^{k-1} \frac{Q_k(\beta)}{k} x^k\right) \Big|_{x=0}, \quad (4)$$

justifying the name generating function.

We now specialize to bosons and derive the recurrence relation for the partition function $Z(N)$ and the ground state occupation number $\eta_0(N, \beta)$. Rewriting (4) and making use of $\Xi(\beta, x)$

$$Z_N(\beta) = \frac{1}{N!} \frac{d^N}{dx^N} \Xi(\beta, 1/x) \Big|_{x=0} \quad (5)$$

we can now write $\eta_i(N, \beta)$ (the number of particles with energy ϵ_i) as

$$\begin{aligned} \eta_i(N, \beta) &= -\frac{1}{\beta} \frac{\partial}{\partial \epsilon_i} \ln Z_N(\beta) \\ &= \frac{1}{\beta} \frac{1}{Z_N(\beta)} \frac{\partial}{\partial \epsilon_i} \frac{1}{N!} \frac{d^N}{dx^N} \Xi(\beta, 1/x) \Big|_{x=0} \end{aligned}$$

Noting that

$$\begin{aligned} \frac{\partial}{\partial \epsilon_i} \Xi(\beta, 1/x) &= \Xi(\beta, 1/x) \sum_{j=1}^{\infty} \frac{\partial}{\partial \epsilon_i} \left(\frac{Q_j(\beta)}{j} x^j \right) \\ &= \Xi(\beta, 1/x) \sum_{j=1}^{\infty} (-1)^j \beta e^{-j\beta\epsilon_i} x^j \end{aligned}$$

and interchanging the order of differentiation we get

$$\eta_i(N, \beta) = \frac{1}{Z_N(\beta)} \frac{1}{N!} \frac{d^N}{dx^N} \Xi(\beta, 1/x) \sum_j e^{-j\beta\epsilon_i} x^j \Big|_{x=0}$$

Since x is set to 0, we need to differentiate x^j j times, which gives $j!$ and there are $\binom{N}{j}$ choices how to do this. So we get

$$\begin{aligned} \eta_i(N, \beta) &= \frac{1}{Z_N(\beta)} \frac{1}{N!} \sum_j e^{-j\beta\epsilon_i} \binom{N}{j} j! \frac{d^{N-j}}{dx^{N-j}} \exp\left(\sum_k \frac{Q_k(\beta)}{k} x^k\right) \Big|_{x=0} \end{aligned}$$

Finally, using (4) we get

$$\eta_i(N, \beta) = \frac{1}{Z_N(\beta)} \sum_j e^{-j\beta\epsilon_i} Z_{N-j}(\beta) \quad (6)$$

Using (6) we can write:

$$\begin{aligned} \eta_i(N+1, \beta) &= \frac{1}{Z_{N+1}(\beta)} \sum_{k=1}^{N+1} e^{-\beta\epsilon_i} Z_{N+1-k}(\beta) \\ &= \frac{Z_N(\beta)}{Z_{N+1}(\beta)} e^{-\beta\epsilon_i} [1 + \eta_i(N, \beta)] \end{aligned} \quad (7)$$

Summing both side and using that $N+1 = \sum \eta_i(N+1, \beta)$ we get

$$\frac{Z_N(\beta)}{Z_{N+1}(\beta)} = \frac{N+1}{\sum_{i=0}^{\infty} e^{-\beta\epsilon_i} [\eta_i(N, \beta) + 1]} \quad (8)$$

When dealing with a bosons in a d dimensional trap, in order to speed the calculation, we label the levels by their total energy and account for the degeneracy $g(i)$ of level i . If we let α be the label of states by their occupation number and suppose that the states $\eta_\alpha(N, \beta)$ all have energy ϵ_i , then $\eta_i(N, \beta) = \sum^{g(i)} \eta_\alpha(N, \beta)$. Since (7) holds for each state α and $\epsilon_\alpha = \epsilon_i$, upon summing the $g(i)$ equations (7) for each α we get

$$\eta_i(N+1, \beta) = \frac{Z_N(\beta)}{Z_{N+1}(\beta)} e^{-\beta\epsilon_i} [\eta_i(N, \beta) + g(i)] \quad (9)$$

Similarly the recurrence relation for $Z_N(\beta)$ transforms into

$$\frac{Z_N(\beta)}{Z_{N+1}(\beta)} = \frac{N+1}{\sum_{i=0}^{\infty} e^{-\beta\epsilon_i} [\eta_i(N, \beta) + g(i)]} \quad (10)$$

3. ZEROS OF Z

$\Xi(\beta, x)$ can be defined for complex β and is holomorphic. By the mathematical theory of holomorphic functions, $Z_N(\beta)$ is an entire function of β , so by the Weierstrass theorem of canonical products[9],

$$Z(\beta) = \exp(g(\beta)) \prod_k (1 - \frac{\beta}{\beta_k})(1 - \frac{\beta}{\beta_k^*}), \quad (11)$$

where β_k and β_k^* are the zeros of $Z(\beta)$ and $\exp(g(\beta))$ is holomorphic and free of zeros on the plane. The zeros come in pairs because $Z_N(\beta^*) = (Z_N(\beta))^*$ and clearly Z_N does not have zeros on the positive real axis.

By the classification theory of Lee and Yang [1] and Grossmann *et al.* [2], the zeros may approach the real axis as $N \rightarrow \infty$, rendering the free energy of the macroscopic system singular. We focus on the Bose gas, and the above singularity indicates Bose-Einstein condensation. However, the imaginary part of the complex zeros are of physical interest in their own right. In particular, the specific heat $C_V(\beta)$ can be obtained from (11)[7]:

$$C_V(\beta) = C_1(\beta) - \sum_k \left[\frac{k_B \beta^2}{(\beta_k - \beta)^2} + \frac{k_B \beta^2}{(\beta_k^* - \beta)^2} \right], \quad (12)$$

where $C_1(\beta)$ is the contribution from $\exp(g(\beta))$ in (11). In the vicinity of a complex zero β_k ,

$$C_V(\beta) = \tilde{C}_1(\beta) - 2 \frac{\beta^2 [(\beta - \text{Re}\beta_k)^2 + (\text{Im}\beta_k)^2]}{[(\beta - \text{Re}\beta_k)^2 + (\text{Im}\beta_k)^2]^2}. \quad (13)$$

Hence, $\text{Im}\beta_k$ shows how singular the specific heat is near the critical temperature for a finite system. Since $\tau_1 = \min_k |\text{Im}\beta_k|$, $\tau_1(N)$ also indicates how fast the properties of the small system near the phase transition converge to those of the macroscopic system.

4. CLASSIFICATION OF PHASE TRANSITIONS

A classification scheme was presented by Grossmann [2] in which the phase transition is completely classified by two parameters, α and γ which govern the density of zeros. Borrmann *et al.* extended this classification to include small systems. In the Borrmann scheme, the complex zeros near the real axis are used to estimate the density of zeros in the thermodynamic limit. Janke *et al.* [10] suggested another description for small systems. A numerical comparison of these two approaches was done in [11].

Here we outline the approach of Borrmann. If we assume that the zeros near the real axis lie approximately on a line, then we can let ν be the angle between this line and the imaginary axis. If $\beta_k = b_k + i\tau_k$ is the k^{th} closest zero to the real axis, then $\nu = \tan \gamma$ where $\gamma = \frac{b_2 - b_1}{\tau_2 - \tau_1}$. To get a sense of how dense the zeros are, we define the discrete line density ϕ as a function of τ_k

$$\phi(\tau_k) = \frac{1}{2} \left(\frac{1}{|\beta_k - \beta_{k-1}|} + \frac{1}{|\beta_{k+1} - \beta_k|} \right)$$

For small τ , $\phi(\tau)$ can be approximated by $\phi \propto \tau^\alpha$. If we look at the second and third closest zeros, then taking $\ln \phi(\tau_3)/\phi(\tau_2)$ and rearranging we obtain

$$\alpha = \frac{\ln \phi(\tau_3) - \ln \phi(\tau_2)}{\ln \tau_3 - \ln \tau_2}$$

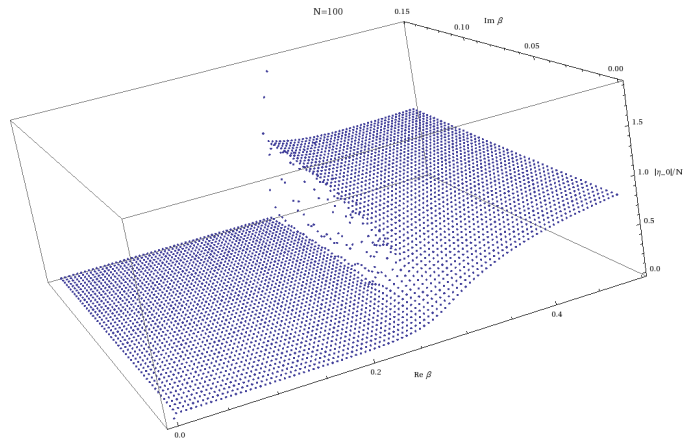


FIG. 1: $\eta_0(100, \beta)/N$ for complex β

In the thermodynamic limit, $\tau_1 \rightarrow 0$ and the classification scheme of Grossmann is recovered. Grossmann showed $\alpha = \gamma = 0$ corresponds to a first order transition, $0 < \alpha < 1$ is second order, and $\alpha > 1$ is higher order. Although for macroscopic phase transitions α is required to be greater than 0, for small systems α can be less than 0. In the Borrmann scheme, a first order transition is therefore defined by $\alpha \leq 0$. The (real) critical temperature of the system is determined by the crossing point with the real axis of the line containing the zeros close to the real axis. So $\beta_{\text{crit}} = b_1 - \gamma\tau_1$. In the thermodynamic limit $\beta_1 \rightarrow \beta_{\text{crit}}$.

5. RESULTS FOR CLASSIFICATION PARAMETERS

In order to classify the phase transition we need to compute the zeros of $Z_N(\beta)$. Noting that the zeros of $Z_N(\beta)$ are the poles of $\eta_0(N, \beta)$, we can instead search for the poles. We compute $Z_N(\beta)$ and $\eta_0(N, \beta)$ recursively through the use of relations (9) and (10). In order to get a sense of the nature of $\eta_0(N, \beta)$, we computed $\eta_0(N, \beta)$ for $d = 3$, $N = 100$ and β taking values in the complex plane. This is shown in figure 1. In the figure, we can clearly see the boundary between the condensed and normal phases. Looking at a cross section with β on the real axis we see a smooth transition between the phases. As the complex part of β is increased, there is an onset of discontinuity in the transition between phases. Also, for complex β we see some of the unphysical values when $\eta_0(N, \beta) > 1$. This was to be expected, as there should be poles for $\eta_0(N, \beta)$ for complex β . Although we do not have enough data points to see the poles, we can still get the impression that, in the language of [8], the poles “radiate” onto the real axis. As the radiation is over a range of temperatures, the occupation numbers

on the real axis are smoothed out.

We now describe our algorithm for finding the classification parameters. The difficulty is locating the zeros that are closest to the real axis. Since Z is sometimes very small, it is easier to instead find the poles of $\eta_0(N, \beta)$. In order to search for the pole of η_0 that is closest to the real axis we utilize the maximum principle of holomorphic functions. By the maximum principle, $|\eta_0|$ cannot have local maxima in the domain where η_0 is holomorphic. Therefore, it suffices to search for the local maximum of $|\eta_0|$ that is closest to the positive real axis. The results for different dimensions are shown in Figure. 2. The results are fit by a power law $\tau_1 = N^{-\rho}$, and the values of the critical exponent ρ are listed in Table 1. In Figure 2. we see that as N increases the nearest pole to the real axis keeps moving closer toward the real axis. Thus the jump in ground state occupation number for β on the real axis keeps increasing, with the pole approaching the real axis as N approaches infinity.

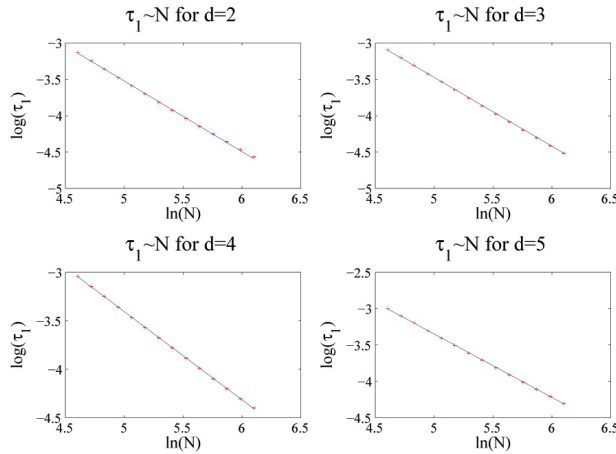


FIG. 2: $\tau_1(N)$ for different dimensions

TABLE I: The critical exponent ρ in different dimensions

d	2	3	4	5
ρ	0.970 ± 0.001	0.946 ± 0.001	0.910 ± 0.001	0.872 ± 0.001

The result for $d = 3$ for τ_1 agrees with [7]. It can be seen that all the ρ for a dimensions 2 – 5 are close to 1 and depend only weakly on d .

Having found τ_1 it is not difficult to compute the other two classification parameters α and γ . We have done this for $d = 3$ (shown in Figure 3.) and the results agree with [7].

6. RENORMALIZATION GROUP

We now give an outline of a renormalization group scheme to compute the exponent ρ . We compute Z_{bN} from (3) ($b > 1$ is an integer):

$$Z_{bN}(\beta) = \frac{1}{2\pi i} \int_C \exp\left(\sum_{k \in \mathbb{N}} \frac{Q_k(\beta)}{k} x^k\right) x^{bN-1} dx.$$

We make the change of variables $x' = x^b$ and $k' = k/b$ to obtain that

$$Z_{bN}(\beta) = \frac{1}{2\pi i} \int_{bC} \exp\left(\sum_{k' \in \frac{1}{b}\mathbb{N}} \frac{Q_{k'b}(\beta)}{k'b} x'^{k'}\right) x'^{N-1} dx'. \quad (14)$$

A recurrence relation can be found if we can find a $\tilde{\beta}$ such that

$$\sum_{k' \in \frac{1}{b}\mathbb{N}} \frac{Q_{k'b}(\beta)}{k'b} \langle x'^{k'} \rangle = \sum_{k \in \mathbb{N}} \frac{Q_k(\tilde{\beta})}{k} \langle x'^k \rangle, \quad (15)$$

since then $Z_{bN}(\beta) = Z_N(\tilde{\beta})$. In particular, if $\beta = a\tilde{\beta} - c$, then $\rho = -\ln a / \ln b$. We note that $Q_{k'b}(\beta) = Q_{k'}(b\beta)$ by definition. Hence, if we take the rudimentary approximation that the summand on the left hand side of (15) remains constant for $k-1 < k' \leq k$, we have $\beta = \tilde{\beta}/b$, so $\rho = 1$. However, the fixed point of β must arise from a correction term to this approximation, which should depend only weakly on β . The detailed renormalization group calculation based on (14) and (15) is beyond the scope of this paper.

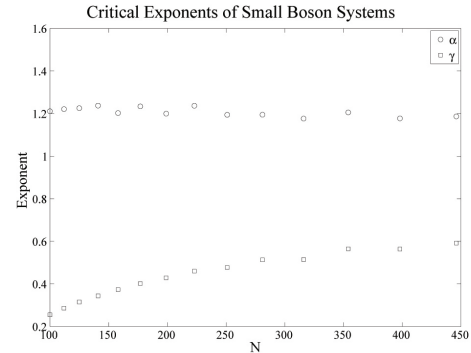


FIG. 3: Classification parameters α and γ versus the number of particles in the $d = 3$ harmonic trap.

7. CONCLUSION

Using the ideas of Yang and Lee and Grossmann *et al.* we have looked at the zeros in the complex temperature plane of the canonical partition function of Bose-Einstein condensate in a trap of dimensions 2–5. By looking at τ_1 as a function of N we are able to see how the true phase

transition is approached in the limit $N \rightarrow \infty$. Looking at the zeros of Z in the complex temperature plane has given a way to understand the development of a phase

transition and link the phase transitions of small systems with phase transitions of macroscopic systems.

-
- [1] C.N. Yang and T. Lee, Phys. Rev. 97, 404 (1952); 87, 410 (1952).
 - [2] S. Grossmann and W. Rosenhauer, Z. Phys. 207, 138 (1967); 218, 437 (1969); S. Grossmann and V. Lehmann, Z. Phys. 218, 449 (1969).
 - [3] M. H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Science 269, 198 1995.
 - [4] D. M. Stamper-Kurn, M.R. Andrews, A.P Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, W. Ketterle, Phys. Rev. Lett. 80, 2027 (1998).
 - [5] P. Navez *et al.*, Phys. Rev. Lett. 79, 1789 (1997).
 - [6] P. Borrmann, *et al.*, Phys. Rev. A. 60, 1519 (1999).
 - [7] P. Borrmann, *et al.*, Phys. Rev. Lett. 84, 3511 (2000).
 - [8] P. Borrmann, *et al.*, Phys. Rev. A. 64, 013611 2001.
 - [9] L. Ahlfors, *Complex Analysis* (McGRAW-HILL, New York, 1979).
 - [10] W. Kanke, R. Kenna, J. Stat. Phys. 102, 1211 (2001).
 - [11] N. A. Alves, J. P. N. Ferrite, U. H. E. Hansmann, Phys. Rev. E. 65, 036110 (2002).
 - [12] O.G. Mouritsen *Computer Studies of Phase Transitions and Critical Phenomena* (Springer-Verlag, Berlin, 1984).