On the Virial Series of the Ideal Bose-Einstein Gas

W. H. J. FUCHS¹

Cornell University, Ithaca, New York

Communicated by C. TRUESDELL

The virial series of the ideal Bose-Einstein gas has been considered by B. WIDOM [2]. In particular he investigated the radius of convergence of this series. The mathematical problem involved is the following. If

$$(1) \quad \begin{aligned} z &= z(\zeta) = \sum_{n=1}^{\infty} n^{-\frac{3}{2}} \zeta^n \\ w &= w(\zeta) = \sum_{n=1}^{\infty} n^{-\frac{5}{2}} \zeta^n, \end{aligned}$$

then near the origin

$$(2) \quad w = \sum_{n=1}^{\infty} a_n z^n.$$

It is required to find the radius of convergence of (2). WIDOM proved

$$\frac{1}{2}e^{\frac{3}{2}} = 0.257 \dots \leq R \leq \infty$$

and conjectured $R = \infty$.

I shall prove

$$\textbf{Theorem.} \quad 12.56 \approx 4\pi \leq R \leq \sum_{n=1}^{\infty} n^{-\frac{3}{2}} + 8\pi \approx 27.73.$$

These estimates are obtained by the application of two lemmas:

Lemma 1. *If the function $z(\zeta)$ defined by (1) can be continued analytically throughout a domain D of the ζ -plane (or of a Riemann surface over the ζ -plane)*

¹This research was supported by the United States Air Force under contract No. AF18(600)-685 monitored by the Office of Scientific Research.

containing $\zeta = 0$, but no other point above the origin of the ζ -plane, and if $z = z(\zeta)$ maps D on a schlicht domain E of the z -plane, then $w = w(\zeta)$ is a regular function of z in E .

In particular R is at least as large as the radius of the largest circle with center at $z = 0$ whose interior lies entirely in E .

Proof. Near $\zeta = 0$

$$(3) \quad \frac{dw}{dz} = \frac{dw}{d\zeta} \cdot \frac{d\zeta}{dz} = \frac{z}{\zeta} \cdot \frac{d\zeta}{dz}.$$

By the assumptions of the lemma the right hand side is a single-valued, analytic function of z for z in E . Hence dw/dz is regular in E , and consequently w is regular in E .

Lemma 2. If $z = z(\zeta)$ assumes the same value twice in a domain D of the ζ -plane containing $\zeta = 0$ (or in a domain D on the Riemann surface of $z(\zeta)$ containing the point $\zeta = 0$, $z(\zeta) = \sum n^{-1} \zeta^n = 0$), then R is less than the upper bound of $|z(\zeta)|$ in D .

Proof. Under the assumptions on D there are two distinct points of D , ζ_0 and ζ_0^* , such that

$$z_0 = z(\zeta_0) = z(\zeta_0^*).$$

We may also assume that $dz/d\zeta \neq 0$ at ζ_0 and ζ_0^* . For, if $dz/d\zeta(\zeta_0) = 0$ to start with, then one can always find new choices of the couple ζ_0, ζ_0^* close to ζ_0 for which the condition on the derivatives is satisfied. Since $dz/d\zeta \neq 0$, we can solve the equations

$$z = z(\zeta) = z(\zeta^*)$$

for ζ and ζ^* as functions of z in the neighborhood of z_0 in such a way that $\zeta(z_0) = \zeta_0$; $\zeta^*(z_0) = \zeta_0^*$. If we assume that $R \geq |z(\eta)|$ ($\eta \in D$), then (3) holds for all $\zeta \in D$. In particular

$$\frac{z(\zeta)}{\zeta} \cdot \frac{d\zeta}{dz} = \frac{z(\zeta^*)}{\zeta^*} \frac{d\zeta^*}{dz}.$$

near $z = z_0$. Or, since $z(\zeta) = z(\zeta^*)$,

$$\frac{1}{\zeta} \frac{d\zeta}{dz} = \frac{1}{\zeta^*} \frac{d\zeta^*}{dz}.$$

Integration gives

$$\zeta^*(z) = a\zeta(z).$$

By analytic continuation this equation must be true for all $\zeta \in D$, i.e.

$$z(\zeta) = z(a\zeta).$$

Lemma 3 below shows that all branches of the many-valued function $z(\zeta)$ have branch-points at $\zeta = 1$ and are regular everywhere else except possibly at 0 and ∞ . Hence we must have $a = 1$. But then $\zeta^* \equiv \zeta$, $z(\zeta^*) \equiv z(\zeta)$, and this contradicts the assumption that ζ and ζ^* are two distinct points of D . This shows that the assumption $R \geq |z(\eta)|$ ($\eta \in D$) is impossible, and the lemma is proved.

In order to utilise these two lemmas we need some facts about $z(\zeta)$. They are special cases of theorems about the functions $\sum_{n=1}^{\infty} n^{-s} \zeta^n$ whose proof can be found in [1].

Lemma 3. *In the ζ -plane with a cut along the positive real axis from 1 to ∞ the function*

$$\varphi(\zeta) = \frac{2}{\sqrt{\pi}} \zeta \int_0^{\infty} \frac{t^{\frac{1}{2}} dt}{e^t - \zeta}$$

represents a direct analytic continuation of the power series for $z(\zeta)$ (i.e. $\varphi(\zeta) = \sum n^{-\frac{3}{2}} \zeta^n$ for $|\zeta| < 1$). $\varphi(\zeta)$ can be continued analytically across the cut along the real axis. If $\varphi_+(\zeta)$ represents the result of continuing $\varphi(\zeta)$ along a path $\mathcal{C}$ which does not cross the negative real axis, starts from ζ and returns to ζ after encircling $\zeta = 1$ once in the positive sense, then

$$\varphi_+(\zeta) = \varphi(\zeta) + 4\sqrt{\pi} (-\log \zeta)^{\frac{1}{2}}.$$

This result is valid in the ζ -plane with a cut from 0 to $-\infty$ along the negative real axis and with another cut from 1 to $+\infty$ along the positive real axis. The many-valued function $(-\log \zeta)^{\frac{1}{2}}$ is determined by the conditions

$$|\Im(\log \zeta)| < \pi; \quad |\arg(-\log \zeta)| < \pi.$$

Similarly, for continuation along a path encircling $\zeta = 1$ in the negative sense

$$\varphi_-(\zeta) = \varphi(\zeta) + 4\sqrt{\pi} (-\log \zeta)^{\frac{1}{2}}.$$

Lemma 4. *If $|\arg(-\zeta)| \leq \pi$, then for large $|\zeta|$*

$$\varphi(\zeta) \sim -\frac{4(\log(-\zeta))^{\frac{1}{2}}}{3\sqrt{\pi}}.$$

When only the leading term is retained, this gives

$$\varphi(\zeta) \sim -\frac{4}{3\sqrt{\pi}} (\log |\zeta|)^{\frac{1}{2}}.$$

Proof of the lower estimate. I define first a portion Δ of the Riemann surface of $z(\zeta)$: Δ has three sheets. Sheet I is a large circle $|\zeta| < K$ with a cut along the positive real axis from 1 to ∞ . Sheets II and III are circles $|\zeta| < K$ with small circles $|\zeta| < \delta$ removed and with cuts from $\zeta = \delta$ to ∞ along the positive real axis. Each cut has an 'upper edge' (which can be reached from the half-plane $\Im(\zeta) > 0$) and a 'lower edge'. The connections between the sheets are as follows:

Every point $\zeta = x$ of the lower edge of sheet I is identified with the point $\zeta = x$ of the upper edge of II. Similarly the upper edge of I and the lower edge of III are identified.

If the function $z(\zeta) = \varphi(\zeta)$ is continued from sheet I into the upper half-plane of sheet II, its value at a point ζ will be

$$\varphi_+(\zeta) = \varphi(\zeta) + 4\sqrt{\pi}(-\log \zeta)^{\frac{1}{2}} \quad (0 < \arg \zeta < \pi),$$

by Lemma 3.

Hence in sheet II the continuation of φ is

$$\varphi_+(\zeta) = \varphi(\zeta) + 4\sqrt{\pi}(-\log \zeta)^{\frac{1}{2}} \quad (0 < \arg \zeta < 2\pi).$$

Similarly continuation into sheet III leads to

$$\varphi_-(\zeta) = \varphi(\zeta) + 4\sqrt{\pi}(-\log \zeta)^{\frac{1}{2}} \quad (-2\pi < \arg \zeta < 0).$$

On the segment $\delta < \zeta < 1$ the values of the function on the upper edge of sheet II and the lower edge of sheet III agree, so that we can join these two edges together. The resulting Riemann domain will be our Δ .

Next I show that every value z_0 in $|z| < 4\pi$ is assumed exactly once by $z(\zeta)$ in Δ by using the 'argument principle':

The number of solutions of $z(\zeta) = z_0$ ($\zeta \in \Delta$) is equal to $(2\pi)^{-1} \cdot (\text{variation of } \arg(z(\zeta) - z_0) \text{ as } \zeta \text{ describes the boundary of } \Delta \text{ once in the positive sense})$.

The boundary of Δ consists of the 'upper edge' of sheet III ($\arg \zeta = -2\pi$) from δ to K , the circle $|\zeta| = K$ described three times in the positive sense (in sheets III, I, II) the 'lower edge' of sheet II ($\arg \zeta = 2\pi$) described from K to δ and the circle $|\zeta| = \delta$ described in the negative sense twice (in sheets II and III).

From the integral representation of $\varphi(\zeta)$ in Lemma 3 it follows that for ζ real, $\zeta > 1$ and on the 'upper edge' of the cut in the ζ -plane

$$\varphi(\zeta) = \text{P. V.} \frac{2}{\pi^{\frac{1}{2}}} \zeta \int_0^\infty \frac{t^{\frac{1}{2}} dt}{e^t - \zeta} + \lim_{\rho \rightarrow 0} \frac{2}{\pi^{\frac{1}{2}}} \int_{K_\rho} \frac{\zeta t^{\frac{1}{2}} dt}{e^t - \zeta},$$

where K_ρ is a semicircle in the lower half plane of radius ρ , center $t = \log \zeta$. The first part of the formula on the right hand side is real, the second part is $2\sqrt{\pi}i \cdot (\text{residue of } \zeta t^{\frac{1}{2}}/(e^t - \zeta) \text{ at } \log \zeta)$.

Hence for real $\zeta > 1$ on the 'upper edge'

$$\Im(\varphi(\zeta)) = 2\sqrt{\pi}i (\log \zeta)^{\frac{1}{2}} > 0.$$

Now I can show that $|z(\zeta)| > 4\pi$ as ζ moves along the straight line boundary of sheet III. Here

$$z(\zeta) = \varphi_+(\zeta) = \varphi(\zeta) + 4\sqrt{\pi}(-\log \zeta + 2\pi i)^{\frac{1}{2}}.$$

If $0 < \zeta < 1$, $0 < \varphi(\zeta)$ and $\Re(-\log \zeta + 2\pi i)^{\frac{1}{2}} > 0$. Hence

$$|z(\zeta)| > 4\pi |(-\log \zeta + 2\pi i)^{\frac{1}{2}}| > 4\pi(2\pi)^{\frac{1}{2}} > 4\pi.$$

If $1 \leq \zeta$, then

$$\begin{aligned} |z(\zeta)| &\geq \Im(z(\zeta)) \geq 4\sqrt{\pi}\Im((- \log \zeta + 2\pi i)^{\frac{1}{2}}) \\ &> 4\sqrt{\pi}\Im(2\pi i)^{\frac{1}{2}} = 4\pi. \end{aligned}$$

The expressions for $z(\zeta)$ also show that $\Im(z(\zeta)) > 0$ on the straight line boundary of sheet III.

Near $\zeta = \delta$

$$\varphi_+(\zeta) \sim 4(-\pi \log \zeta)^{\frac{1}{2}},$$

which is a large positive number. Near $\zeta = K$

$$\varphi_+(\zeta) \sim -\frac{4}{3\pi^{\frac{1}{2}}}(\log K)^{\frac{3}{2}},$$

which is a large negative number. From collecting all these data it follows that $\arg(z(\zeta) - z_0)$ increases approximately by π as ζ varies from δ to K along the boundary of sheet III for every z_0 with $|z_0| \leq 4\pi$. On the circles $|\zeta| = K$

$$z(\zeta) \sim -\frac{4}{3\pi^{\frac{1}{2}}}(\log K)^{\frac{3}{2}},$$

and on the circles $|\zeta| = \delta$ in sheets II and III

$$z(\zeta) \sim 4(-\pi \log \delta)^{\frac{1}{2}}.$$

Therefore $\arg(z(\zeta) - z_0)$ does not change much as ζ describes the circular parts of the boundary of Δ . The curve described by $z(\zeta)$ as ζ varies along the straight-line boundary of sheet II is obtained from the image of the other straight-line boundary by reflexion in the real axis. The variation of $\arg(z(\zeta) - z_0)$ along this line is again about π . Hence, by the argument principle every z_0 with $|z_0| < 4\pi$ is assumed exactly once in Δ . The lower bound for R now follows from Lemma 1 by choosing as D the sub-domain of Δ whose image in the z -plane is the circle $|z| < 4\pi$.

Proof of the upper estimate. Let $\mathcal{C}_x$ be the path from $\zeta = 0$ to $\zeta = 1 - \epsilon$ along the real axis, then looping round $\zeta = 1$ once in the positive sense along a small circle with center at 1 and finally back to the point x , $0 < x < 1 - \epsilon$. If $\varphi(\zeta)$ is continued along $\mathcal{C}_x$, then it takes on the (real) value $\varphi_+(x)$ which tends to $+\infty$ as $x \rightarrow 0$.

Let $\mathcal{D}$ be the following path: From $\zeta = 0$ to $1 - \epsilon$; in a small loop round $\zeta = 1$ anti-clockwise; along $|\zeta| = 1 - \epsilon$ two complete revolutions anti-clockwise; again round $\zeta = 1$ anti-clockwise and finally round $|\zeta| = 1 - \epsilon$ clockwise.

The various values assumed by $z(\zeta)$ at a point of $|\zeta| = 1 - \epsilon$, ($0 < \arg \zeta < \pi$) are

$$\varphi(\zeta) + 4\sqrt{\pi}(-\log \zeta)^{\frac{1}{2}},$$

$$\begin{aligned} & \varphi(\zeta) + 4\sqrt{\pi}(-\log \zeta - 2\pi i)^{\frac{1}{2}}, \\ & \varphi(\zeta) + 4\sqrt{\pi}\{(-\log \zeta - 2\pi i)^{\frac{1}{2}} + (-\log \zeta + 2\pi i)^{\frac{1}{2}}\}. \end{aligned}$$

$$\text{In } |\zeta| \leq 1$$

$$|\varphi(\zeta)| \leq \varphi(1) = \sum_{n=1}^{\infty} n^{-\frac{3}{2}} \approx 2.612,$$

and, for $\zeta = e^{i\alpha}$, $0 < \alpha < \pi$

$$\begin{aligned} |(-\log \zeta)^{\frac{1}{2}}|^2 &< |(-\log \zeta - 2\pi i)^{\frac{1}{2}}|^2 < |(-\log \zeta - 2\pi i)^{\frac{1}{2}} + (-\log \zeta + 2\pi i)^{\frac{1}{2}}|^2 \\ &= |(\alpha + 2\pi)^{\frac{1}{2}} e^{-\pi i/4} + (2\pi - \alpha)^{\frac{1}{2}} e^{\pi i/4}|^2 \\ &= 2\pi + \alpha + 2\pi - \alpha \\ &= 4\pi. \end{aligned}$$

Similarly $|z(\zeta)|$ can be estimated for ζ in the lower half-plane.

Hence for ζ close to the path $\mathfrak{D}$ and ϵ very small

$$(4) \quad |z(\zeta)| < \varphi(1) + 8\pi + \delta,$$

where $\delta > 0$ can be chosen arbitrarily small. At the endpoint of $\mathfrak{D}$

$$z(\zeta) = \varphi(1 - \epsilon) + 4\sqrt{\pi}\{(-\log(1 - \epsilon) - 2\pi)^{\frac{1}{2}} + (-\log(1 - \epsilon) + 2\pi i)^{\frac{1}{2}}\}$$

is arbitrarily close to $\varphi(1) + 8\pi$, if ϵ is sufficiently small. We can now apply Lemma 2 to a domain consisting of narrow strips round the paths $\mathfrak{D}$ and $\mathfrak{C}_x$ where x is chosen as the largest number between 0 and 1 for which $\varphi_+(x) = \varphi(1) + 8\pi$. Values close to this number are taken on twice in the domain and therefore (4) implies $R \leq \varphi(1) + 8\pi = 27.73$.

We remark finally that the function $w(z)$ is regular in a domain containing the whole real axis. This follows from Lemma 1, if we observe that the argument used to prove $R \geq 4\pi$ can also be used to show that we may take for E in Lemma 1 a domain symmetrical about the real axis bounded by two curves, one above the real axis, the other below.

These results indicate that the singularities of the Virial Expansion have no close connection with the phenomenon of condensation.

The author wishes to thank Professor M. KAC for bringing the problem to his notice and for discussing it with him.

BIBLIOGRAPHY

1. BARNES, E. W., Proc. London Math. Soc. (2) **4**, 284 (1906).
2. WIDOM, B., The Virial Series of the Bose-Einstein Gas, Phys. Rev. **96**, 16-17 (1954).