D-dimensional Bose Gases and the W Function

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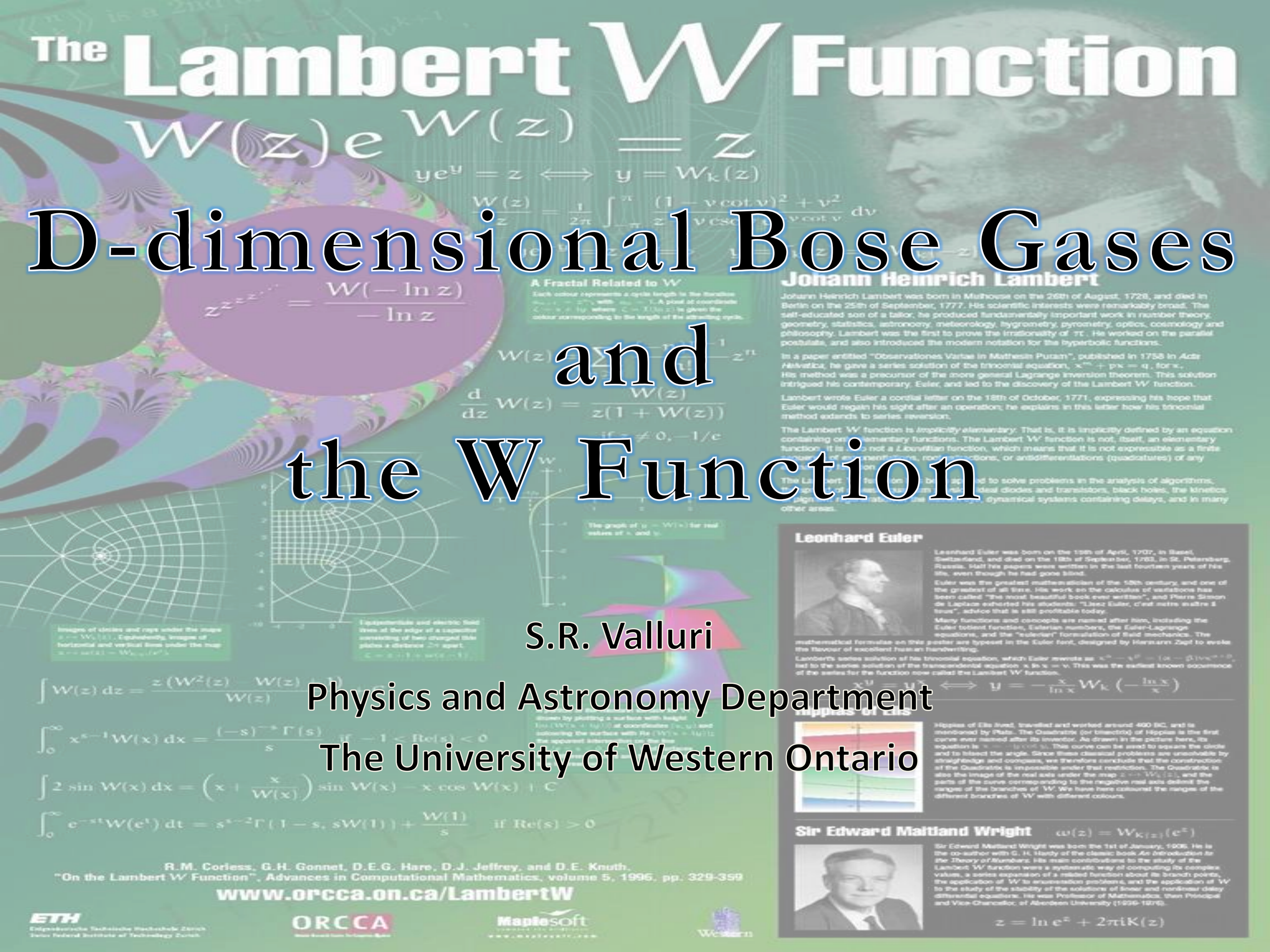

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1. The Lambert W function and quantum statistics, Journal of Mathematical Physics, **50**, 2009
2. D-Dimensional Bose gases and the Lambert W function accepted with minor revisions, February 2010

Introduction

- The applications of the W function (hereafter mostly referred to as the W function) to D-dimensional Bose gases are presented in this talk.

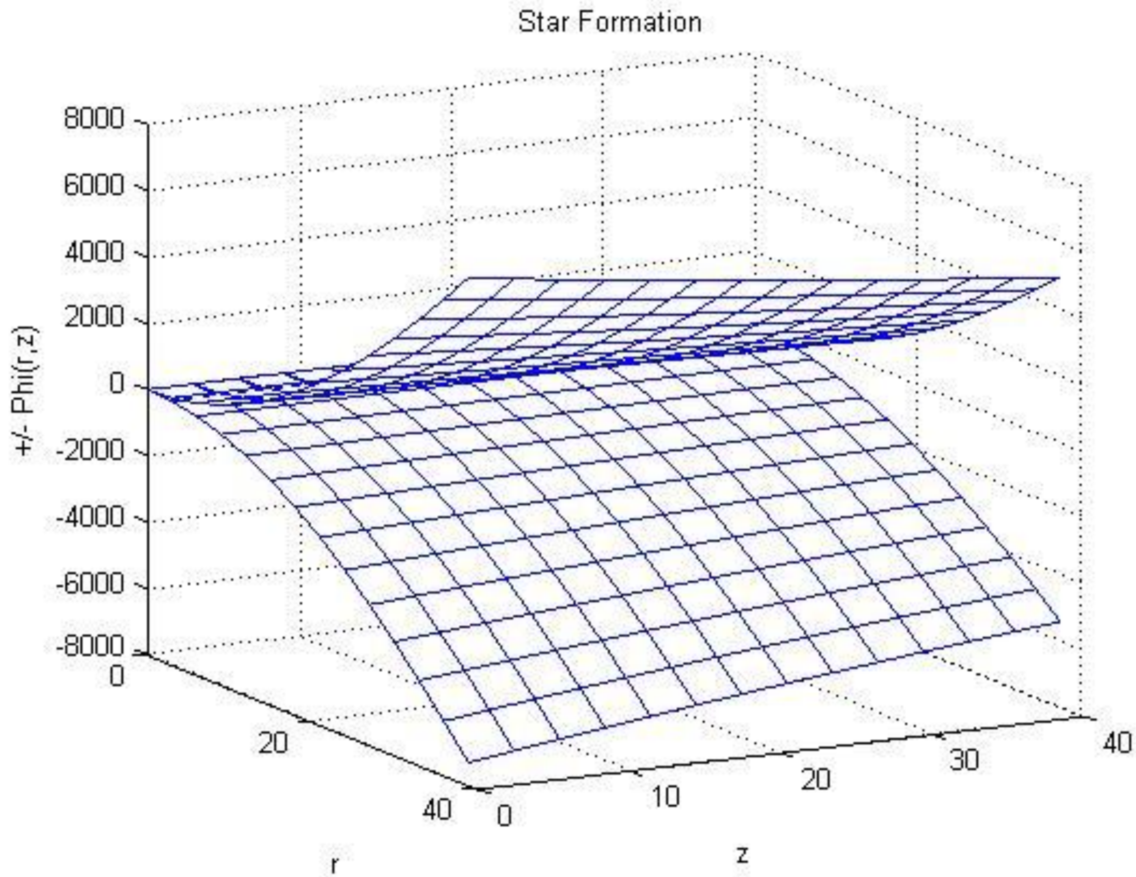
- The low temperature *T* behavior of free ideal Bose gases is considered in 2, 3 and 4 dimensions.

Contents

1. Applications of the W function

- Enumerating search trees
- Solutions to transcendental equations
- Analytic solutions to solar cell parameters
- Wien’s displacement law
- Fringing fields of a parallel plate capacitor

The **W function** has the potential to provide solutions to problems that have previously not been solved analytically, as well as uncovering novel and interesting properties of previously solved problems.



A function Phi(r,z) that can be used to generate magnetic field lines in terms of the Lambert W

2. The W function

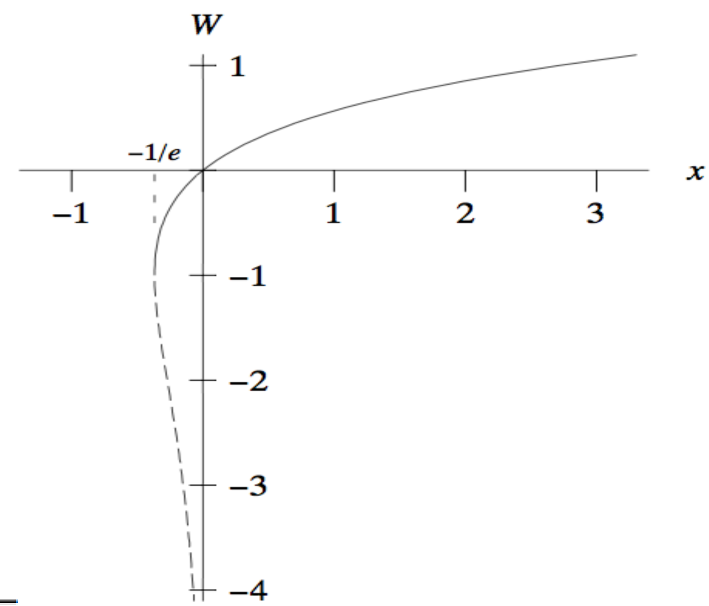
The W function is defined as the multivalued function which solves the following equation:

$$W(z)\exp(W(z)) = z \qquad\qquad z \in \mathbb{C}\ ,$$

(1)

or, equivalently, as the multivalued inverse of the function

$$f\ :\ z\ \to\ ze^{z}$$



For real argument, at most two solutions:

- W_0 (solid line) is the principal branch
- W_{-1} (dashed line)

$$W_0(z) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!} z^n = z - z^2 + \frac{3}{2} z^3 - \ldots.$$

(2)

Two families of transcendental equations appear in statistical mechanics, applied mathematical and physics problems.

Type 1: $$x^n + B\ln x + C = 0\ . \qquad (3)$$

where $n, B, C \in \mathbb{C}$ not depending on x and $n, B \neq 0$. Then

$$\frac{n}{B}x^n + n\ln x = -\frac{nC}{B} \Rightarrow \frac{n}{B}x^n e^{\frac{n}{B}x^n} = \frac{n}{B}e^{-\frac{nC}{B}}\ .$$

Type 2: $$x = \left[\frac{B}{n}W_j\left(\frac{n}{B}\exp\left(-\frac{nC}{B}\right)\right)\right]^{1/n}\ . \qquad (4)$$

$$x^n\ln x + Bx^n + C = 0\ . \qquad (5)$$

$$n\ln x + nB = -Cnx^{-n} \Rightarrow -Cne^{nB} = -Cnx^{-n}e^{-Cnx^{-n}}\ .$$

$$x = \left[-\frac{1}{Cn}W_j\left(-Cne^{nB}\right)\right]^{-1/n}\ . \qquad (6)$$

3A. Thermodynamic Functions

$$\bar{n}_{BE} = -\frac{1}{\mathcal{Z}_{BE}}\frac{\partial \mathcal{Z}_{BE}}{\partial x} = \frac{1}{e^{\beta(\epsilon-\mu)} - 1}\ , \quad (7)$$

$$\bar{n}_{FD} = -\frac{1}{\mathcal{Z}_{FD}}\frac{\partial \mathcal{Z}_{FD}}{\partial x} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}\ , \quad (8)$$

where $x = \beta(\epsilon - \mu)$,

ϵ is the energy,

μ is the chemical potential,

$\beta = 1/kT$, T is the temperature,

and k is Boltzmann constant.

$\mathcal{Z}$ is the Grand Partition Function

$\bar{n}_{BE}, \bar{n}_{FD}$ **are the distributions for number of particles over different quantum energy states at T for systems of bosons and fermions.**

3B. Quantum Statistics

1. Fermi-Dirac

2. Bose-Einstein

- In this work we will present applications of the W function to free ideal Bose gases.

- We represent the number of particles N, entropy S, pressure P, chemical potential μ, and energy U using the Z grand partition function:

$$N = kT\frac{\partial(\ln \mathcal{Z})}{\partial\mu}\ , \quad S = -k\frac{\partial(T\ln \mathcal{Z})}{\partial T}\ , \quad P = kT\frac{\partial(\ln \mathcal{Z})}{\partial V}$$

$$\mu = -kT\frac{\partial(\ln \mathcal{Z})}{\partial N}\ , \quad U = kT^2\frac{\partial(\ln \mathcal{Z})}{\partial T}\ .$$

- The thermodynamic quantity that gives most insight into the nature of BEC is the fugacity

$$z = e^{\beta\mu}$$

- In the limit where all bosons are in the ground state, the fugacity approaches unity.

4. Two, Three and Four Dimensional Ideal Bose Gases

- The reduced particle density for a Bose gas in D dimensions is given in terms of a polylogarithm of order related to the dimension. The result is:

$$\rho\lambda^D = Li_{m+1}(z) \ , \qquad (9)$$

- Where $Li_{m+1}(z)$ is the polylogarithm of order m + 1, m=D/2 -1 and D is the dimension, $z = e^{\beta\mu}$ is the fugacity of the system, $\lambda = \sqrt{2\pi\hbar^2/kTM}$ is the de-Broglie wavelength, M is the mass of the constituent particles, and the quantity $\rho\lambda^D$ is referred to as the reduced particle density.

The analysis presented here relies on an expansion of the polylogarithms about $z = 1$.

If m=0,1,2, (D=2,4,6,), as $z \rightarrow 1$,

$$Li_{m+1} = \frac{(-1)^{m+1}}{\Gamma(m+1)} \left(\ln\frac{1}{z}\right)^m \left(\ln\ln\left(\frac{1}{z}\right) - \psi(m+1) + \psi(1)\right) + \sum_{r=0(r\neq m)}^{\infty} \frac{\zeta(m+1-r)(\ln z)^r}{r!},$$

(10)

Where $\zeta(s)$ is the Riemann Zeta Function,

$\Gamma(s)$ is the Gamma Function, and

$\psi(s)$ (also referred to as the Digamma Function) is the logarithmic derivative of the Gamma Function.

4A. Chemical Potential

- In $D = 2$ and $D = 4$ dimensions, from $\rho\lambda^D = Li_{m+1}(z)$,

the reduced particle densities are

$$\rho\lambda^2 = Li_1(z), \quad D = 2 \ , \qquad \text{(11a)}$$

and

$$\rho\lambda^4 = Li_2(z), \quad D = 4 \qquad \text{(11b)}$$

Two dimensional case:

$m = 0 \longrightarrow$ the logarithmic derivatives cancel.

as r increases the summation become small in the following:

$$Li_{m+1} = \frac{(-1)^{m+1}}{\Gamma(m+1)} \left(\ln\frac{1}{z}\right)^m \left(\ln\ln\left(\frac{1}{z}\right) - \psi(m+1) + \psi(1)\right) + \sum_{r=0(r\neq m)}^{\infty} \frac{\zeta(m+1-r)(\ln z)^r}{r!} ,$$

From the previous eqn. and $\rho\lambda^4 = Li_2(z)$, $\quad D = 4$ the reduced particle density near $z = 1$ is

$$\rho\lambda^2 = Li_1(z) \approx -\ln\ln(1/z) + \zeta(0)\ln z \quad D = 2 \qquad (12)$$

which can be rewritten as

$$x - 2\ln x - 2\rho\lambda^2 = 0 \,, \quad x = -\ln z$$

using the fact that $\zeta(0) = -1/2$

Hence this (12) is of the form (3) with $n = 1$, $B = -2$ and $C = -2\rho\lambda^2$ so that its solution is given by (4),

$$x = -\ln z = -2\, W_j \left[-\frac{1}{2} \exp\left(-\left(\frac{-2\rho\lambda^2}{-2} \right) \right) \right]^{1/1} \qquad (13)$$

and by the definition of z we have $\mu = -kTx$, then,

$$\mu = 2kTW_j \left(-\frac{1}{2} e^{-\rho\lambda^2} \right) \,, \quad \lambda = \sqrt{2\pi\hbar^2/kTM} \,, \quad D = 2 \,.$$

y is the argument of the W function

$$y \to 0 \Rightarrow W_0(y) \to 0 \text{ and } W_{-1}(y) \to -\infty.$$

if μ is given in terms of W_0 then

$$T \to 0 \Rightarrow \lambda \to \infty \Rightarrow \mu \to \ 0$$

$$W_0(0) = 0,$$

Whereas if μ is expressed in terms of W_{-1} (z), then $\beta\mu \to -\infty$

Since we are interested in region $z \approx 1$ we only consider the solution in terms of W_0.

$$\mu = -kT\sum_{n=1}^{\infty}\left(\frac{n}{2}\right)^{n-1}\frac{e^{-n\rho\lambda^2}}{n!}\ . \qquad (14)$$

Based on this expression we have the following results in 2-D:

- For real μ, treating $\rho\lambda^2$ as an independent variable, the series (14) has a radius of convergence $R = 1 - \ln 2$.Within the circle of convergence, $|\mu| < 2kT$. Also, μ has a branch point at $\rho\lambda^2 = 1 - \ln 2$ and a branch cut along the negative real axis:

$$\rho\lambda^2 \in (-\infty, R).$$

- For real values of μ , condensation occurs when $e^{-\rho\lambda^2} \longrightarrow 0$, as expected in two dimensions. This is in agreement $T \longrightarrow 0$, with the result obtained by Lee.

Return to chemical potential in 4-D

$D = 4$, $m = 1$,

$$\rho\lambda^4 = \ln\left(\frac{1}{z}\right)\left(\ln\ln\left(\frac{1}{z}\right) - \psi(2) + \psi(1)\right) + \zeta(2)\ , \qquad (15)$$

Where $\psi(2) = \psi(1) + 1$, $\psi(1) = -C$, C is Euler's constant .

Equivalently,

$$x\ln(x) - x + (\zeta(2) - \rho\lambda^4) = 0 \quad x = -\ln z\ , \qquad (16)$$

with $n = 1$, $B =$ -1 and $C = (\zeta(2) - \rho\lambda^4)$.

- Therefore the solution to (15) using $\zeta(2) = \pi^2/6.$

$$x = -\ln z = \left[-\frac{1}{(1)(\zeta(2) - \rho\lambda^4)} W_j\left(-(\zeta(2) - \rho\lambda^4)(1)\exp((1)(-1))\right)\right]^{-1/1},$$

$$= \left(\rho\lambda^4 - \frac{\pi^2}{6}\right)\left[W_j\left(\left[\rho\lambda^4 - \frac{\pi^2}{6}\right]e^{-1}\right)\right]^{-1}$$

By the definition of $W(z)$, $W(z)^{-1} = \exp(W(z))/z$, so:

$$\mu = -kTx = -kT\exp\left(W_j\left(\frac{1}{e}\left[\rho\lambda^4 - \frac{\pi^2}{6}\right]\right) + 1\right) \qquad (17)$$

In general, (17) allows for the possibility of a complex chemical potential. By choosing ***j* = 0** or ***j* = −1** the chemical potential is real.

For real branches of W , a solution exists if:

$$W_j\left[e^{-1}\left(\rho\lambda^4-(\pi^2/6)\right)\right] \to -\infty,$$

which is only possible if $j = -1$ and $e^{-1}\left(\rho\lambda^4 - \frac{\pi^2}{6}\right) \to 0.$

Recalling that: $\lambda = \sqrt{2\pi\hbar^2/(MkT)},$

We have:

$$T_c = \sqrt{\frac{24\hbar^4\rho}{k^2M^2}} = \frac{2\hbar^2\sqrt{6\rho}}{kM}\ . \qquad (18)$$

By definition,

$$W_{-1}(z) \in \mathbb{R} \iff z \in [-1/e, 0).$$

This constraint can be expressed in terms of T_c by noting that in our case it is equivalent to

$$T \in [(\pi/\sqrt{6+\pi^2})T_c, T_c) \approx [0.789T_c, T_c).$$

For real values, T must be within about 80% and 100% T_c

4B. Pressure

Pressure P is a function of the chemical potential.

$$\frac{\rho}{kT} = \frac{\partial P}{\partial \ln z}$$

As a **polylogarithm,** order of pressure P depends on the dimension. Hence, for two-dimensional case:

$$\frac{P}{kT} = \frac{2}{\lambda^2} Li_2(z) \quad D = 2$$

<u>Note:</u> Volume and Temperature are held fixed

ρ is the number density

z is the fugacity

N is the number of particles

Two-Dimensional Case of Ideal Bose Gas

The pressure around $z = 1$ is expressed as:

$$\frac{P}{kT} \approx \frac{2}{\lambda^2}\left[\ln\left(\frac{1}{z}\right)\left(\ln\left(\ln\left(\frac{1}{z}\right)\right) - 1\right) + \frac{\pi^2}{6}\right] .$$

The fact that $\ln z = (1/kT)\mu$, leads to:

$$\frac{P}{kT} \approx \frac{2}{\lambda^2}\left[-2W_j\left(-\frac{1}{2}e^{-\rho\lambda^2}\right)\left(\ln\left(-2W_j\left(-\frac{1}{2}e^{-\rho\lambda^2}\right)\right) - 1\right) + \frac{\pi^2}{6}\right]$$

$$\ln(-2W_j(y)) + W_j(y) = \ln 2 + \ln(-y) \ .$$

Thus, pressure of a two-dimensional gas is:

$$\frac{P}{kT} \approx \frac{4}{\lambda^2}\left[W_j\left(-\frac{1}{2}e^{-\rho\lambda^2}\right)\right]^2 + \frac{4(\rho\lambda^2+1)}{\lambda^2}W_j\left(-\frac{1}{2}e^{-\rho\lambda^2}\right) + \frac{\pi^2}{3\lambda^2} \ , \quad D = 2.$$

When W_0 is very small,

$$\frac{P}{kT} = \frac{4(\rho\lambda^2+1)}{\lambda^2}W_0\left(-\frac{1}{2}e^{-\rho\lambda^2}\right) + \frac{\pi^2}{3\lambda^2} \ , \quad D = 2$$

<u>Note:</u> As limit $T \rightarrow 0$ ($\lambda \rightarrow \infty$), right hand side $\rightarrow$ 0

- Using series expansion for W_0 about $z = 0$, series expansion for pressure about $\rho\lambda^2 >> 1$ is:

$$\boxed{\frac{P}{kT} = -\frac{2(\rho\lambda^2+1)}{\lambda^2}\sum_{n=1}^{\infty}\left(\frac{n}{2}\right)^{n-1}\frac{e^{-n\rho\lambda^2}}{n!} + \frac{\pi^2}{3\lambda^2} \ , \quad D = 2}$$

Four-Dimensional Case of Ideal Bose Gas

Pressure is expressed as: $\frac{P}{kT} = \frac{2}{\lambda^3} Li_3(z) \quad D = 4$

As mentioned above,

$$Li_{m+1} = \frac{(-1)^{m+1}}{\Gamma(m+1)} \left(\ln \frac{1}{z}\right)^m \left(\ln \ln \left(\frac{1}{z}\right) - \psi(m+1) + \psi(1)\right) + \sum_{r=0 (r \neq m)}^{\infty} \frac{\zeta(m+1-r)(\ln z)^r}{r!}$$

pressure is related to fugacity ***z*** by:

$$\frac{P}{kT} = \frac{2}{\lambda^3} \left[-\frac{1}{\Gamma(3)} \left(\ln \left(\frac{1}{z}\right)\right)^2 \left(\ln \ln \left(\frac{1}{z}\right) - \psi(3) + \psi(1)\right) + \zeta(3) + \zeta(2) \ln z \right]$$

and by neglecting ln z terms of order ≥2 :

$$\frac{P}{kT} \approx \frac{2\zeta(3)}{\lambda^3} + \frac{2\zeta(2)}{\lambda^3} \ln z$$

Using solution

$$\mu = -kTx = -kT \exp\left(W_j\left(\frac{1}{e}\left[\rho\lambda^4 - \frac{\pi^2}{6}\right]\right) + 1\right)$$

equation of state for free ideal Bose gas near z =1 and D=4 is:

$$\boxed{\frac{P}{kT} = \frac{2\zeta(3)}{\lambda^3} - \frac{\pi^2}{3\lambda^3} \exp\left(W_{-1}\left(\frac{1}{e}\left[\frac{\pi^2}{6} - \rho\lambda^4\right]\right) + 1\right)}$$

Conclusions

- **New representations for chemical potential μ, P, T of Bose Gas**
  - Relationship between chemical potential and T in terms of W function in two, three, four dimensions
  - Branch cuts of chemical potential in two dimensions
  - Chemical Potential and Decay in a BEC
  - Series Expansion in terms of quantity exp $(-\varrho\lambda^2)$ with D=2
  - Expression for small T below condensation T

    Real Values for chemical potential for $T \in [0.789T_c, T_c)$
  - Equation of state in BEC regime

- **W function and analysis of BEC of trapped ideal Bose gas**
  - Condensate T with D=1, expressed in terms of N.
  - Chemical Potential with D=2, express in terms of T and N.

- **High T expansions for P and ρ of hard-core bosons, D=1**
  - Radius of Convergence, Coefficients of Mayer expansions differ from Tonk gas
  - Temperature, chemical potential, pressure in low temperature analysis

- **Applications of Type 1 and Type 2 equations to Bose-Einstein and Maxwell-Boltzmann systems at high temperatures.**
  - Convergence of different statistics in classical unit
  - Complex chemical potential and temperature
  - Incomplete complex analysis for ideal Bose at D=2 & D=4 near condensation
  - Further study on branch cuts, singularities of the thermodynamic functions.

- **Applications of W function**
- **Obtaining several special solutions of W function in classical and non-classical limits**
- **Bose and Lambert are no more but Bosons and The Lambert W will live for ever.**