The Sommerfeld Expansion

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06.07.2007, revisited 15.07.2007

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Abstract

This Document will provide a proof for the Sommerfeld expansion formula used for integrals involving the Dirac Distribution and a sufficiently well behaved but otherwise arbitrary function. Also included from my previous works is the derivation for the formula connecting the values of the Riemann-Zeta function for even integers with the Bernoulli numbers, which is used within the proof. The main result will be equation (23/24) on page 6. Also two different motivations/ways for the reshaping of the integral, the first step in the derivation, are provided and an additional treatment in terms of fugacity is given.

1 The Sommerfeld Expansion

1.1 Transformation of the Integral

1.1.1 First Derivation of the Intermediate Result

Following and correcting a discussion in L. Landau, E. Lifshitz: Statistical Physics Part I, 3rd Edition, page 169/170. Notation is slightly changed for convenience.
We want to approximate the following integral for a function $f(\epsilon)$ such that the integral I converges.

$$I = \int_0^\infty \frac{f(\epsilon)}{e^{\frac{(\epsilon-\mu)}{k_B T}}+1}\mathrm{d}\epsilon \tag{1}$$

We transform the integral by a change of coordinates via
$(\epsilon-\mu)/(k_B T)=z$, $\epsilon = k_B T z+\mu$, $\mathrm{d}\epsilon/\mathrm{d}z = k_B T$ or $\mathrm{d}\epsilon = k_B T\mathrm{d}z$

$$\begin{aligned} I &= \int_{-\mu/(k_B T)}^\infty \frac{f(k_B T z+\mu)}{e^z+1}k_B T\mathrm{d}z \\ &= k_B T\int_{-\mu/(k_B T)}^0 \frac{f(k_B T z+\mu)}{e^z+1}\mathrm{d}z + k_B T\int_0^\infty \frac{f(k_B T z+\mu)}{e^z+1}\mathrm{d}z \\ &= k_B T\int_0^{\mu/(k_B T)} \frac{f(\mu-k_B T z)}{e^{-z}+1}\mathrm{d}z + k_B T\int_0^\infty \frac{f(k_B T z+\mu)}{e^z+1}\mathrm{d}z \end{aligned} \tag{2}$$

Now, since $\frac{1}{e^{-z}+1}=\frac{e^z}{e^z+1}=1-\frac{1}{e^z+1}$ we split the first integral and hence:

$$I = k_B T\int_0^{\mu/(k_B T)} f(\mu-k_B T z)\,\mathrm{d}z - k_B T\int_0^{\mu/(k_B T)} f(\mu-k_B T z)\frac{1}{e^z+1}\mathrm{d}z + k_B T\int_0^\infty \frac{f(k_B T z+\mu)}{e^z+1}\mathrm{d}z$$

Transforming the first integral back via $\epsilon=\mu-k_B T z$, $\mathrm{d}\epsilon/\mathrm{d}z=-k_B T$ or $\mathrm{d}z=\mathrm{d}\epsilon/(k_B T)$

$$I = \int_0^\mu f(\epsilon)\mathrm{d}\epsilon - k_B T\int_0^{\mu/(k_B T)} \frac{f(\mu-k_B T z)}{e^z+1}\mathrm{d}z + k_B T\int_0^\infty \frac{f(k_B T z+\mu)}{e^z+1}\mathrm{d}z \tag{3}$$

Now comes the first approximation (up to now this was all exact and simply manipulation of the integral to bring it into a suggestive form). We replace the upper limit in the second integral with infinity. This is legitimate since $\mu/(k_B T)\approx E_F/(k_B T) >> 1$ and the integral is rapidly convergent:

$$I \approx \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + k_B T\int_0^\infty \frac{f(\mu+k_B T z)-f(\mu-k_B T z)}{e^z+1}\mathrm{d}z \tag{4}$$

We now Taylor-Expand the function f around μ and obtain:

$$
\begin{aligned}
I &\approx \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + k_B T \int_0^\infty \left\{ \sum_{n=0}^\infty \frac{f^{[n]}(\mu)}{n!}(k_B T z)^n - \frac{f^{[n]}(\mu)}{n!}(-k_B T z)^n \right\} \frac{1}{e^z+1}\mathrm{d}z \\
&= \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + k_B T \sum_{n=1}^\infty \int_0^\infty \frac{f^{[2n-1]}(\mu)}{(2n-1)!} 2(k_B T)^{(2n-1)} \frac{z^{2n-1}}{e^z+1}\mathrm{d}z \\
&= \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + \sum_{n=1}^\infty \frac{f^{[2n-1]}(\mu)}{(2n-1)!} 2(k_B T)^{2n} \int_0^\infty \frac{z^{2n-1}}{e^z+1}\mathrm{d}z \\
&= \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + \sum_{n=1}^\infty \frac{f^{[2n-1]}(\mu)}{(2n-1)!} 2(k_B T)^{2n} I_{2n} \qquad (5)
\end{aligned}
$$

1.1.2 Seocond Derivation of the Intermediate Result

A further approch to reach this result is presented in Reference [2]. In this document though, the notation is altered from the reference to be conform with the first discussion. Consider again the following integral:

$$I = \int_0^\infty \frac{f(\epsilon)}{e^{\frac{(\epsilon-\mu)}{k_B T}}+1}\mathrm{d}\epsilon = \int_0^\infty f(\epsilon)D(\epsilon)\mathrm{d}\epsilon \qquad (6)$$

where $D(\epsilon)$ is the Dirac Distribution. Define $F(x)$ by

$$F(\epsilon) = \int_0^\epsilon f(\epsilon')\mathrm{d}\epsilon' \qquad (7)$$

We now integrate by parts the former integral:

$$I = [D(\epsilon)F(\epsilon)]_0^\infty - \int_0^\infty D'(\epsilon)F(\epsilon)\mathrm{d}\epsilon \qquad (8)$$

The first term vanishes since $D(\infty)=0$ and $F(0)=0$. Hence we are left with

$$I = -\int_0^\infty D'(\epsilon)F(\epsilon)\mathrm{d}\epsilon \qquad (9)$$

Now, when evaluating this integral the important point that Sommerfeld made is to note is that D' is sharply peaked at $\epsilon=\mu\approx E_F$, particularly at low temperatures T. Thus we expand $F(\epsilon)$ around $\epsilon=\mu$:

$$F(\epsilon) = \sum_{n=0}^\infty \frac{F^{[n]}(\mu)}{n!}(\epsilon-\mu)^n \qquad (10)$$

This transfroms the integral into the following convergent series:

$$I = -\sum_{n=0}^\infty \frac{1}{n!}F^{[n]}(\mu)\int_0^\infty D'(\epsilon)(\epsilon-\mu)^n\mathrm{d}\epsilon \qquad (11)$$

Yet again, change of variable via $z=(\epsilon-\mu)/k_B T, \quad \mathrm{d}z/\mathrm{d}\epsilon = 1/(k_B T)$ brings us to the form:

$$I \approx -\sum_{n=0}^\infty \frac{1}{n!}F^{[n]}(\mu)\int_{-\infty}^\infty \frac{-e^z}{(e^z+1)^2}(k_B T z)^n\mathrm{d}z = \sum_{n=0}^\infty \frac{(k_B T)^n F^{[n]}(\mu)}{n!}\int_{-\infty}^\infty \frac{e^z}{(e^z+1)^2}z^n\mathrm{d}z \qquad (12)$$

The first step in the above sequence was replacing the lower bound by $-\infty$ which is legitimate since D' goes to zero quickly away from $\epsilon=\mu$. This step is done to realize that odd integers n do not contribute in the sum obtained last (later the limit of integration will be set back to 0): $\frac{e^z}{(e^z+1)^2} = \left(\frac{1}{2\cosh(z/2)}\right)^2$ is an even function (cosh is an even function), and hence when multiplied by an odd function (z^{2n+1}) and integrated over the real line gives zero! Since the integral for $n=0$ is 1 we are left with:

$$\begin{aligned} I &\approx F(\mu) + \sum_{n=1}^{\infty} \frac{(k_B T)^{2n} F^{[2n]}(\mu)}{(2n)!} \left(2\int_0^{\infty} \frac{e^z}{(e^z+1)^2} z^{2n} \mathrm{d}z\right) \\ &= F(\mu) + \sum_{n=1}^{\infty} \frac{(k_B T)^{2n} F^{[2n]}(\mu)}{(2n)!} 2\left\{\left[\frac{-1}{e^z+1} z^{2n}\right]_0^{\infty} + \int_0^{\infty} (2n)\frac{z^{2n-1}}{e^z+1}\right\} \\ &= F(\mu) + \sum_{n=1}^{\infty} \frac{2(k_B T)^{2n} F^{[2n]}(\mu)}{(2n-1)!} I_{2n} \end{aligned} \tag{13}$$

Now we replace F by f to get:

$$I = \int_0^{\infty} f(\epsilon)D(\epsilon)\mathrm{d}\epsilon \approx \int_0^{\mu} f(\epsilon)\mathrm{d}\epsilon + \sum_{n=1}^{\infty} \frac{2(k_B T)^{2n} f^{[2n-1]}(\mu)}{(2n-1)!} I_{2n} \tag{14}$$

Note how equation (5) and (14) coincide.

1.2 The Missing Integral-Factor I_{2n}

The integral I_{2n} can be computed using the definitions of the Riemann-Zeta function $\zeta(x)$ and the Gamma function $\Gamma(x)$ and furthermore the Geometric Series (see Appendix):

$$\begin{aligned} \Gamma(x) &= \int_0^{\infty} z^{x-1} e^{-z} \mathrm{d}z \\ \zeta(x) &= \sum_{n=1}^{\infty} \frac{1}{n^x} \\ \sum_{k=1}^{\infty} z^k &= \frac{z}{1-z} \quad \text{for} \quad |z| \le 1 \end{aligned}$$

With those tools at hand we are ready to compute the following integral:

$$\begin{aligned} I_x &= \int_0^{\infty} \frac{z^{x-1}}{e^z+1} \mathrm{d}z = \int_0^{\infty} z^{x-1} e^{-z} \left(\frac{1}{1+e^{-z}}\right) \mathrm{d}z \\ &= \int_0^{\infty} z^{x-1} e^{-z} \left(\sum_{n=0}^{\infty} (-e^{-z})^n\right) \mathrm{d}z = \int_0^{\infty} \sum_{n=0}^{\infty} (-1)^n z^{x-1} e^{-(1+n)z} \mathrm{d}z \end{aligned} \tag{15}$$

Now we change the variable of integration to transform the inner integral into the Gamma function:
$z' = (1+n)z, \quad z = \frac{1}{(1+n)} z', \quad \mathrm{d}z'/\mathrm{d}z = (1+n) \quad \text{or} \quad \mathrm{d}z = \frac{1}{(1+n)} \mathrm{d}z'$

$$\begin{aligned} I_x &= \int_0^{\infty} \sum_{n=0}^{\infty} (-1)^n \left(\frac{z'}{n+1}\right)^{x-1} e^{-z'} \frac{1}{n+1} \mathrm{d}z' = \int_0^{\infty} \sum_{n=1}^{\infty} (-1)^{n-1} z^{x-1} e^{-z} \frac{1}{n^x} \mathrm{d}z \\ &= \sum_{n=1}^{\infty} (-1)^{n+1} \frac{1}{n^x} \Gamma(x) = \left(\frac{2^x-2}{2^x}\right) \zeta(x)\Gamma(x) = \left(1-2^{1-x}\right) \zeta(x)\Gamma(x) \end{aligned} \tag{16}$$

Here I used equation (94) to relate the infinite sum over n to the Riemann-Zeta function:

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)^p} = \frac{2^p-2}{2^p} \zeta(p) \quad \text{for} \quad p > 1$$

..to express the sum within the lengthy term in terms of the Riemann-Zeta function.
If $x = 2k$ is an even integer we can use the explicit expression derived later, see equation (84), for $\zeta(2n)$ in terms of Bernoulli numbers B_n:

$$(-1)^{k+1}(2\pi)^{2k}\frac{B_{2k}}{2(2k)!} = \zeta(2k) \quad \text{for} \quad k \in \text{Integers}$$

This gives for I_{2k} using equation (16) the following expression:

$$\begin{aligned} I_{2k} &= \int_0^\infty \frac{z^{2k-1}}{e^z+1}\mathrm{d}z = \left(\frac{2^{2k}-2}{2^{2k}}\right)\left((-1)^{k+1}2^{2k}\pi^{2k}\frac{B_{2k}}{2(2k)!}\right)(2k-1)! \\ &= \left(2^{2k}-2\right)(-1)^{k+1}\frac{\pi^{2k}B_{2k}}{4k} = \left(\frac{2^{2k-1}-1}{2k}\right)(-1)^{k+1}\pi^{2k}B_{2k} \end{aligned} \tag{17}$$

1.2.1 A Special Case and a Similar Integral

This section derives additional interesting results which are not needed for the Sommerfeld expansion, but easily derived at this point with the previous setup.
For $x = 1$ we go one step back to get a result and note that the Taylor expansion of $\ln(1+x)$ reads:

$$\begin{aligned} \ln(1+x) &= \sum_{n=1}^\infty (-1)^{n+1}\frac{x^n}{n} \quad \text{for} \quad |x| \le 1 \\ \ln(2) &= \sum_{n=1}^\infty (-1)^{n+1}\frac{1}{n} \end{aligned} \tag{18}$$

Thus we get for I_1 using an intermediate step in equation (16):

$$I_1 = \int_0^\infty \frac{1}{e^z+1}\mathrm{d}z = \sum_{n=1}^\infty (-1)^{n+1}\frac{1}{n}\Gamma(1) = \ln(2) \tag{19}$$

An other intergral of interest can be computed using the same technique as in the previous section:

$$\begin{aligned} I_x &= \int_0^\infty \frac{z^{x-1}\mathrm{d}z}{e^z-1} = \int_0^\infty z^{x-1}\left(\frac{1}{e^z-1}\right)\mathrm{d}z = \int_0^\infty z^{x-1}\left(e^{-z}\sum_{n=0}^\infty \left(e^{-z}\right)^n\right)\mathrm{d}z \\ &= \sum_{n=0}^\infty \int_0^\infty z^{x-1}e^{-(1+n)z}\mathrm{d}z \end{aligned} \tag{20}$$

Analogous to the previous treatment we change the variable of integration to transform the inner integral into the Gamma function: $z' = (1+n)z, \quad z = \frac{1}{(1+n)}z', \quad \mathrm{d}z'/\mathrm{d}z = (1+n) \quad \text{or} \quad \mathrm{d}z = \frac{1}{(1+n)}\mathrm{d}z'$

$$\begin{aligned} I_x &= \sum_{n=0}^\infty \int_0^\infty \left(\frac{z'}{1+n}\right)^{x-1} e^{-z'}\frac{1}{1+n}\mathrm{d}z' = \sum_{n=1}^\infty \int_0^\infty z^{x-1}e^{-z}\frac{1}{n^x}\mathrm{d}z \\ &= \int_0^\infty z^{x-1}e^{-z}\sum_{n=1}^\infty \frac{1}{n^x}\mathrm{d}z = \Gamma(x)\zeta(x) \end{aligned} \tag{21}$$

For even integers this becomes:

$$\begin{aligned} I_{2n} &= \Gamma(2n)\zeta(2n) = (2n-1)!(-1)^{n+1}(2\pi)^{2n}\frac{B_{2n}}{2(2n)!} \\ &= \frac{(-1)^{n+1}(2\pi)^{2n}B_{2n}}{4n} = \frac{(-4)^{n-1}\pi^{2n}B_{2n}}{n} = \int_0^\infty \frac{z^{2n-1}\mathrm{d}z}{e^z-1} \end{aligned} \tag{22}$$

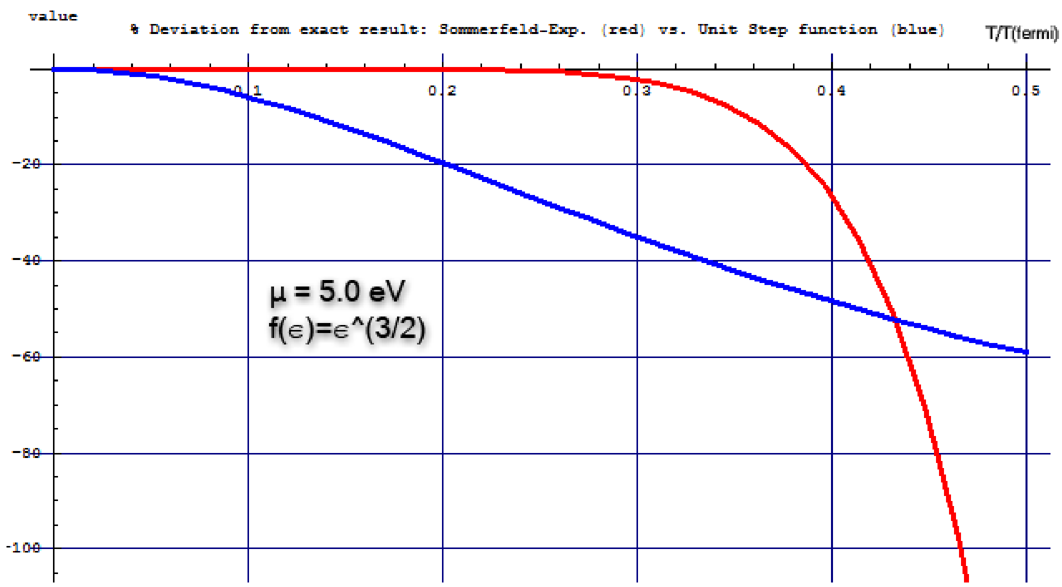
1.3 The Result

Going back to our original problem we find from equation (14)/(15) and (17):

$$\begin{aligned}
I &= \int_0^\infty \frac{f(\epsilon)}{e^{\frac{(\epsilon-\mu)}{k_B T}}+1}\mathrm{d}\epsilon \;=\; \int_0^\infty f(\epsilon)D(\epsilon)\mathrm{d}\epsilon \\
&\approx \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + \sum_{n=1}^{\infty}\frac{f^{[2n-1]}(\mu)}{(2n-1)!}2(k_B T)^{2n}\left\{\left(\frac{2^{2n-1}-1}{2n}\right)(-1)^{n+1}\pi^{2n}B_{2n}\right\} \\
&= \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + \sum_{n=1}^{\infty}\frac{f^{[2n-1]}(\mu)}{(2n)!}(k_B T)^{2n}\left(2^{2n}-2\right)(-1)^{n+1}\pi^{2n}B_{2n} \qquad (23) \\
&= \int_0^\mu f(\epsilon)\mathrm{d}\epsilon + \frac{\pi^2(k_B T)^2 f'(\mu)}{6} + \frac{7\pi^4(k_B T)^4 f'''(\mu)}{360} + \qquad (24) \\
&\quad \frac{31\pi^6(k_B T)^6 f'''''(\mu)}{15120} + \frac{127\pi^8(k_B T)^8 f'''''''(\mu)}{604800} + \ldots
\end{aligned}$$

This is the **final result**, where in equation (24) the Bernoulli Numbers derived in the next section were used (see recurrence formula and table 1 for B_n in the Section 2.2). The formula is an **asymptotic approximation** and not a convergent series, as L. Landau points out (see Reference [1]) and is seen in the picture below .
This is equivalent to the approximation of the Fermi-Dirac distribution by the Unit-Step-function and terms involving derivatives of the generalized Dirac Delta Distribution $\delta(x)$:

$$D(\epsilon) = \frac{1}{e^{\frac{(\epsilon-\mu)}{k_B T}}+1} \approx \Theta(\mu-\epsilon) + \sum_{n=1}^{\infty}\frac{\delta^{[2n-1]}(\mu-\epsilon)}{(2n)!}(k_B T)^{2n}\left(2^{2n}-2\right)(-1)^{n}\pi^{2n}B_{2n}$$



Sidenote: Setting $k_B = 1$ and $T = 1$ we can **generalize the result** for $\eta >> 1$:

$$\begin{aligned}
\int_0^\infty \frac{f(x)}{e^{x-\eta}+1}\mathrm{d}x &\approx \int_0^\eta f(x)\mathrm{d}x + \sum_{n=1}^{\infty}\frac{f^{[2n-1]}(\eta)}{(2n)!}\left(2^{2n}-2\right)(-1)^{n+1}\pi^{2n}B_{2n} \\
&= \int_0^\eta f(x)\mathrm{d}x + \frac{\pi^2}{6}f'(\eta) + \frac{7\pi^4}{360}f'''(\eta) + \ldots
\end{aligned}$$

1.4 Application: $\mu \longleftrightarrow E_F$ and $c_V \longleftrightarrow E_F$

Again following Reference [2] we derive the dependence of μ on Temperature T:
From the lecture we know the density of states for the free electron gas in a box in terms of Fermi-Energy E_F and the total number N of electrons is:

$$g(\epsilon) = \frac{3}{2}\frac{N}{E_F}\left(\frac{\epsilon}{E_F}\right)^{1/2} \qquad N = \int_0^\infty g(\epsilon)D(\epsilon)\mathrm{d}\epsilon \quad \Rightarrow \quad E_F^{3/2} = \frac{3}{2}\int_0^\infty \epsilon^{1/2}D(\epsilon)\mathrm{d}\epsilon \tag{25}$$

Now we see that for the Sommerfeld Approximation we should set $f(\epsilon) = \epsilon^{1/2}$ and carry along all the prefactors. We thus get the following (where the general form of the derivative was observed):

$$\begin{aligned}
E_F^{3/2} &\approx \frac{3}{2}\left(\int_0^\mu \epsilon^{1/2}\mathrm{d}\epsilon + \sum_{n=1}^\infty \frac{\mathrm{d}\left(\epsilon^{1/2}\right)(\mu)}{(2n)!\,\mathrm{d}\epsilon^{2n-1}}(k_BT)^{2n}\left(2^{2n}-2\right)(-1)^{n+1}\pi^{2n}B_{2n}\right) \\
&= \mu^{3/2} + \sum_{n=1}^\infty \frac{3}{2}\left(\frac{(|3+4(n-2)|)!!}{(2n)!\,2^{2n-1}}\mu^{-\frac{5+4(n-2)}{2}}\right)(k_BT)^{2n}\left(2^{2n}-2\right)(-1)^{n+1}\pi^{2n}B_{2n} \\
&= \mu^{3/2}\left(1 + \sum_{n=1}^\infty 3\left(\frac{(|4n-5|)!!}{(2n)!}\mu^{-2n}\right)(k_BT)^{2n}\left(1-2^{1-2n}\right)(-1)^{n+1}\pi^{2n}B_{2n}\right) \\
&= \mu^{3/2} + \frac{3}{2}\frac{\pi^2}{6}(k_BT)^2\frac{1}{2}\mu^{-1/2} + \frac{3}{2}\frac{7\pi^4}{360}(k_BT)^4\frac{1}{2}\frac{(-1)}{2}\frac{3}{2}\mu^{-5/2} + \ldots \\
&= \mu^{3/2}\left(1 + \frac{3\pi^2}{24}\left(\frac{k_BT}{\mu}\right)^2 + \frac{7\pi^4}{360}\frac{9}{16}\left(\frac{k_BT}{\mu}\right)^4 + \ldots\right)
\end{aligned} \tag{26}$$

..using the following Power-series expansion

$$(1+x)^n = \sum_{k=0}^\infty \frac{n(n-1)\ldots(n-k+1)}{k!}x^k = \sum_{k=0}^\infty \frac{\Gamma(n+1)}{\Gamma(n-k+1)\Gamma(k+1)}x^k \tag{27}$$

..and keeping in mind $n!! = \frac{n!}{2^{(2n-1)/2}((2n-1)/2)!} = n(n-2)\ldots 1$ for odd integers we get:

$$\begin{aligned}
E_F &\approx \sum_{k=0}^\infty \frac{\Gamma(2/3+1)}{\Gamma(2/3-k+1)\Gamma(k+1)}\left(\sum_{n=1}^\infty 3\left(\frac{(|4n-5|)!!}{(2n)!}\mu^{-2n}\right)(k_BT)^{2n}\left(1-2^{1-2n}\right)(-1)^{n+1}\pi^{2n}B_{2n}\right)^k \\
&= \mu + \frac{\pi^2}{12}\frac{(k_BT)^2}{\mu} + \frac{\pi^4}{180}\frac{(k_BT)^4}{\mu^3} + \ldots \\
&= \mu\left(1 + \frac{\pi^2}{12}\left(\frac{k_BT}{\mu}\right)^2 + \frac{\pi^4}{180}\left(\frac{k_BT}{\mu}\right)^4 + \ldots\right)
\end{aligned} \tag{28}$$

Inversion of this equation to the same order in E_F gives the following result (this can be done by hand, basically comparison of coefficients, but Mathematica's bulit in function *InverseSeries[]* comes in handy here):

$$\mu \approx E_F\left(1 - \frac{\pi^2}{12}\left(\frac{k_BT}{E_F}\right)^2 - \frac{\pi^4}{80}\left(\frac{k_BT}{E_F}\right)^4 - \ldots\right) \tag{29}$$

This whole procedure can be easily implemented in **Mathematica** to find the coefficients up to arbitrary order of $\left(\frac{k_BT}{E_f}\right)$ or $\left(\frac{k_BT}{\mu}\right)$, respectively. (For an alternative way: see Reference [10]).

In a similar way we obtain the specific electronic heat in terms of Fermi energy, making use in the calculation of the formula for μ in terms of E_F which was derived before.

$$u_0 = \int_0^{E_F} g(\epsilon)\,\epsilon\, D(\epsilon)\mathrm{d} \qquad u = \int_0^\infty g(\epsilon)\,\epsilon\, D(\epsilon)\mathrm{d}\epsilon \qquad c_V = \frac{\partial}{\partial T}u \tag{30}$$

Sommerfeld Expansion: Fermi Energy - chemical potential relation

In[240]:=
```
Clear[μ, kB, T, Ef];
uptoN = 10;

EFSeriesNEW =
  FullSimplify[
   Series[
    μ *
     Sum[(Gamma[2 / 3 + 1] / (Gamma[2 / 3 - k + 1] Gamma[k + 1]))
       (Sum[3 (Abs[4 n - 5]) !! / (2 n) ! (1 - 2^(1 - 2 n)) * (-1)^(n + 1) BernoulliB[2 n] * (kB T)^(2 n) π^(2 n) * μ^(-2 n), {n, 1, uptoN}])^k, {k, 0, uptoN}],
    {μ, Infinity, uptoN}]];


Print["EFermi = ", Simplify[(Normal[EFSeriesNEW] / μ)] * μ]
SeriesMu = InverseSeries[EFSeriesNEW, Ef];
Print["μ = ", Simplify[(Normal[SeriesMu] / Ef)] * Ef]
Print["Ef Series coeff. for (kB T/μ)^n are: (format: {n,coeff.,N[coeff.]})",
 Table[{n, Coefficient[Simplify[(Normal[EFSeriesNEW] / μ)], (kB T/μ)^n],
   N[Coefficient[Simplify[(Normal[EFSeriesNEW] / μ)], (kB T/μ)^n], 3]}, {n, 2, uptoN, 2}]]
Print["mu Series coeff. for (kB T/Ef)^n are: (format: {n,coeff.,N[coeff.]})",
 Table[{n, Coefficient[Simplify[(Normal[SeriesMu] / Ef)], (kB T/Ef)^n],
   N[Coefficient[Simplify[(Normal[SeriesMu] / Ef)], (kB T/Ef)^n], 3]}, {n, 2, uptoN, 2}]]
```

Out[135]= EFermi $= \left(1+\frac{1563139\,kB^{10}\pi^{10}T^{10}}{18662400\,\mu^{10}}+\frac{26093\,kB^{8}\pi^{8}T^{8}}{1555200\,\mu^{8}}+\frac{169\,kB^{6}\pi^{6}T^{6}}{25920\,\mu^{6}}+\frac{kB^{4}\pi^{4}T^{4}}{180\,\mu^{4}}+\frac{kB^{2}\pi^{2}T^{2}}{12\,\mu^{2}}\right)\mu$

$\mu = Ef\left(1-\frac{kB^{2}\pi^{2}T^{2}}{12\,Ef^{2}}-\frac{kB^{4}\pi^{4}T^{4}}{80\,Ef^{4}}-\frac{247\,kB^{6}\pi^{6}T^{6}}{25920\,Ef^{6}}-\frac{16291\,kB^{8}\pi^{8}T^{8}}{777600\,Ef^{8}}-\frac{1487\,kB^{10}\pi^{10}T^{10}}{15360\,Ef^{10}}\right)$

Ef Series coeff. for $(\frac{kB\,T}{\mu})$^n are: (format: {n,coeff.,N[coeff.]})

$\left\{\left\{2,\frac{\pi^2}{12},0.822\right\},\left\{4,\frac{\pi^4}{180},0.541\right\},\left\{6,\frac{169\pi^6}{25920},6.27\right\},\left\{8,\frac{26093\pi^8}{1555200},159.\right\},\left\{10,\frac{1563139\pi^{10}}{18662400},7.84\times10^{3}\right\}\right\}$

mu Series coeff. for $(\frac{kB\,T}{Ef})$^n are: (format: {n,coeff.,N[coeff.]})

$\left\{\left\{2,-\frac{\pi^2}{12},-0.822\right\},\left\{4,-\frac{\pi^4}{80},-1.22\right\},\left\{6,-\frac{247\pi^6}{25920},-9.16\right\},\left\{8,-\frac{16291\pi^8}{777600},-199.\right\},\left\{10,-\frac{1487\pi^{10}}{15360},-9.07\times10^{3}\right\}\right\}$

Sommerfeld Expansion: Fermi Energy - electron Heat Capacity relation

In[541]:=
```
Clear[μ, kB, T, Ef];
ArbFunc[ϵ_] := ϵ^(3 / 2);

μIntegral := Integrate[ArbFunc[ϵ], {ϵ, 0, μ}] + Sum[((2^(2 n) - 2) (kB T)^(2 n) π^(2 n) (D[ArbFunc[ϵ], {ϵ, 2 n - 1}] /. ϵ → μ) / (2 n) ! (-1)^(n + 1) BernoulliB[2 n]), {n, 1, 7}];

EAv = (3 N / (2 Ef^(3 / 2)) μIntegral) /. μ → Ef (1 - kB^2 π^2 T^2/(12 Ef^2) - kB^4 π^4 T^4/(80 Ef^4) - 247 kB^6 π^6 T^6/(25920 Ef^6) - 16291 kB^8 π^8 T^8/(777600 Ef^8) - 1487 kB^10 π^10 T^10/(15360 Ef^10));

SeriesEF = Series[EAv, {Ef, Infinity, 7}];
Print["E = ", NSeriesEF = Normal[SeriesEF]]
Print["cv = ", cvSeries = D[NSeriesEF, T] /. Ef -> kB Tf]

Print["cV Series coeff. for kB(T/Tf)^n are: (format: {n,coeff.,N[coeff.]}) ",
 Table[{n, Coefficient[cvSeries, kB (T/Tf)^n], N[Coefficient[cvSeries, kB (T/Tf)^n], 3]}, {n, 1, 5, 2}]]
```

$E = \frac{3\,Ef\,N}{5}+\frac{kB^2 N\pi^2T^2}{4\,Ef}-\frac{3\,kB^4N\pi^4T^4}{80\,Ef^3}-\frac{247\,kB^6N\pi^6T^6}{12096\,Ef^5}-\frac{10367\,kB^8N\pi^8T^8}{259200\,Ef^7}$

$cv = -\frac{10367\,kB\,N\pi^8T^7}{32400\,Tf^7}-\frac{247\,kB\,N\pi^6T^5}{2016\,Tf^5}-\frac{3\,kB\,N\pi^4T^3}{20\,Tf^3}+\frac{kB\,N\pi^2T}{2\,Tf}$

cV Series coeff. for kB$(\frac{T}{Tf})$^n are: (format: {n,coeff.,N[coeff.]}) $\left\{\left\{1,\frac{N\pi^2}{2},4.93\,N\right\},\left\{3,-\frac{3N\pi^4}{20},-14.6\,N\right\},\left\{5,-\frac{247N\pi^6}{2016},-118.\,N\right\}\right\}$

From the Mathematica file we read off the electronic contribution to the **specific heat** in solids predicted by the Sommerfeld-Theory, where $k_B T_F = E_F$:

$$c_V = k_B N \left(\frac{\pi^2}{2} \left(\frac{T}{T_F} \right) - \frac{3\pi^4}{20} \left(\frac{T}{T_F} \right)^3 - \frac{247\pi^6}{2016} \left(\frac{T}{T_F} \right)^5 - \dots \right) \tag{31}$$

1.5 Treatment in Terms of Fugacity / Fermi- and Bose-Functions $f_\nu(z)$, $b_\nu(z)$

In statistical physics it is common to define the fugacity z by $z = e^{\beta\mu} = e^{\mu/(k_B T)}$. The motivation or context, along with the definitions can be found in *IdealQuantumGases.pdf* and the corresponding Mathematica notebook *fermi.nb*, both located on the lecture notes homepage of James J. Kelly on http://www.physics.umd.edu/courses/Phys603/kelly/.

Defined is the **Fermi Function** by the following similar integral:

$$f_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{z^{-1}e^x + 1} \mathrm{d}x \tag{32}$$

For small z, this can be expressed as a power series as mentioned and calculated in the Mathematica file by the program function *Series[]* (Reference [12]). I will derive this expansion by hand in the following lines:

$$\begin{aligned}
f_\nu(z) &= \frac{1}{\Gamma(\nu)} \int_0^\infty x^{\nu-1} \left(\frac{1}{z^{-1}e^x + 1} \right) \mathrm{d}x = \frac{1}{\Gamma(\nu)} \int_0^\infty x^{\nu-1} \left(z e^{-x} \sum_{k=0}^\infty (-z e^{-x})^k \right) \mathrm{d}x \\
&= \frac{z}{\Gamma(\nu)} \sum_{k=0}^\infty (-z)^k \int_0^\infty x^{\nu-1} e^{-x(k+1)} \mathrm{d}x \\
&= \frac{z}{\Gamma(\nu)} \sum_{k=0}^\infty (-z)^k \int_0^\infty \left(\frac{x}{k+1} \right)^{\nu-1} e^{-x} \frac{1}{(k+1)} \mathrm{d}x \\
&= \frac{z}{\Gamma(\nu)} \sum_{k=0}^\infty (-z)^k \Gamma(\nu) \frac{1}{(k+1)^\nu} = -\sum_{k=0}^\infty (-z)^{k+1} \frac{1}{(k+1)^\nu} \\
&= -\sum_{k=1}^\infty \frac{(-z)^k}{k^\nu} \qquad \text{for all } 0 < z < 1, \nu > 0
\end{aligned} \tag{33}$$

The limiting value for $\nu \to \infty$ is seen to be z since in the sum only $k = 1$ will contribute:

$$f_\infty(z) = z \tag{34}$$

also note the following recursive relation, which are useful in handling the fermi-functions:

$$\frac{\partial}{\partial z} f_\nu(z) = \sum_{k=1}^\infty \frac{(-z)^{k-1}}{k^{\nu-1}} = -\frac{1}{z} f_{\nu-1}(z) \Rightarrow z \frac{\partial}{\partial z} f_\nu(z) = -f_{\nu-1}(z) \tag{35}$$

A similar series expansion can be given for BE integrals, the **Bose Function** is definde by:

$$b_\nu(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{x^{\nu-1}}{z^{-1}e^x - 1} \mathrm{d}x \tag{36}$$

It seems as if the Fermi-Functions and the Bose-Functions, which are those kinds of integrals, are defined slightly different depending on the paper or book they appear in. Another definition will appear shortly on the side to see how they convert into each other. The derivation now for the expansion is analogously to the expansion of the Fermi-Function we have seen before:

$$\begin{aligned} b_\nu(z) &= \frac{1}{\Gamma(\nu)}\int_0^\infty x^{\nu-1}\left(\frac{1}{z^{-1}e^x-1}\right)\mathrm{d}x \;=\; \frac{1}{\Gamma(\nu)}\int_0^\infty x^{\nu-1}\left(ze^{-x}\sum_{k=0}^{\infty}\left(ze^{-x}\right)^k\right)\mathrm{d}x \\ &= \frac{1}{\Gamma(\nu)}\sum_{k=0}^{\infty} z^{k+1}\int_0^\infty x^{\nu-1}e^{-x(k+1)}\mathrm{d}x = \frac{1}{\Gamma(\nu)}\sum_{k=0}^{\infty} z^{k+1}\int_0^\infty\left(\frac{x}{k+1}\right)^{\nu-1}e^{-x}\frac{1}{(k+1)}\mathrm{d}x \\ &= \frac{1}{\Gamma(\nu)}\sum_{k=0}^{\infty} z^{k+1}\Gamma(\nu)\frac{1}{(k+1)^\nu} = \sum_{k=0}^{\infty}\frac{z^{k+1}}{(k+1)^\nu} \;=\; \sum_{k=1}^{\infty}\frac{z^k}{k^\nu} \qquad \text{for all } 0<z<1,\ \nu>0 \end{aligned} \tag{37}$$

Also here we note off the following obvious properties:

$$b_\infty(z) = z\,; \qquad \frac{\partial}{\partial z}b_\nu(z) = z b_{\nu-1}(z) \tag{38}$$

This series expansion establishes the useful **relation between** $f_\nu(z)$ **and** $b_\nu(z)$, which can be found in a somewhat **different notation** in Reference [13]. For completeness, since in theoretical applications their notation seems to be common, I will compare them shortly:

$$\begin{aligned} B_p(\eta) &= \frac{1}{\Gamma(p+1)}\int_0^\infty \frac{x^p}{e^{x-\eta}-1}\mathrm{d}x \;\Rightarrow\; B_p(\eta) = b_{p+1}(e^\eta);\ \ \frac{\partial}{\partial\eta}B_{p+1}(\eta) = B_p(\eta);\ \ B_p(\eta) = \sum_{k=1}^{\infty}\frac{e^{k\eta}}{k^{p+1}} \\ F_p(\eta) &= \frac{1}{\Gamma(p+1)}\int_0^\infty \frac{x^p}{e^{x-\eta}+1}\mathrm{d}x \;\Rightarrow\; F_p(\eta) = f_{p+1}(e^\eta);\ \ \frac{\partial}{\partial\eta}F_{p+1}(\eta) = F_p(\eta);\ \ F_p(\eta) = \sum_{k=1}^{\infty}\frac{(-1)^{k+1}e^{k\eta}}{k^{p+1}} \end{aligned}$$

(The two series hold for $\eta < 0$) However, in our notation the relation is derived the following way:

$$f_\nu(z) = -\sum_{k=1}^{\infty}\frac{(-z)^k}{k^\nu} = -\left(\frac{-z}{1^\nu}+\frac{z^2}{2^\nu}-\frac{z^3}{3^\nu}+\ldots\right) = \sum_{k=1}^{\infty}\left(\frac{z^k}{k^\nu}-2\frac{z^{2k}}{(2k)^\nu}\right) = b_\nu(z) - \frac{2}{2^\nu}b_\nu\left(z^2\right) \tag{39}$$

This is of importance since there are numerous different approximations to the Bose-functions as well. Some of them, for example those treated in Reference [13], use **Chebyshev Polynomials** and are extremely good and the series are fastly converging.

Another useful approximation to the Fermi-Function $F_p(\eta)$ is the generalized approximation put forward by Aymerich-Humet, F. Serra-Mestres and J. Millán (See Reference [14]). It is a fit-model approach that is accurate up to a few percent and works over a wide range of η and sensible values of p:

$$\begin{aligned} \Gamma(p+1)F_p(\eta) &\approx \left(\frac{(p+1)\,2^{p+1}}{\left(b+\eta+\left(\left|\eta-b\right|^c+a^c\right)^{1/c}\right)^{p+1}}+\frac{e^{-\eta}}{\Gamma(p+1)}\right)^{-1} \\ a &= \left(1+\frac{15}{4}(p+1)+\frac{1}{40}(p+1)^2\right)^{1/2},\quad b = (1.8+0.61p),\quad c = \left(2+\left(2-\sqrt{2}\right)2^{-p}\right) \end{aligned} \tag{40}$$

In the treatment with the form of the integral given by equation (32), **for large** z, Sommerfeld's lemma is derived in a similar way to the treatments we have seen before, using again the idea of the function being a Unit-Step function to first order and then, this time, adding and substracting corrections, where the error in the approximation comes in here because of changing the limits of the second integral to $-\infty$ in the second line. The hint for this approach is to be found in the Mathematica file *fermi.nb* where the Mathematica function *Series[]* is used again (Reference [12]). I will derive the general formula by hand, where again equation (27) and the equation (17) for I_{2k} are used, listed here once more for convenience:

$$(1+x)^n = \sum_{k=0}^{\infty}\frac{\Gamma(n+1)}{\Gamma(n-k+1)\Gamma(k+1)}x^k\,, \qquad I_{2k} = \left(2^{2k}-2\right)(-1)^{k+1}\frac{\pi^{2k}B_{2k}}{4k}$$

The derivation to the general expansion formula goes like this:

$$
\begin{aligned}
f_\nu(z) &= \frac{1}{\Gamma(\nu)}\int_0^\infty \frac{x^{\nu-1}\mathrm{d}x}{e^{x-\log(z)}+1} \\
&\approx \frac{1}{\Gamma(\nu)}\left\{\int_0^{\log(z)} x^{\nu-1}\mathrm{d}x + \int_{\log(z)}^\infty \frac{x^{\nu-1}}{e^{x-\log(z)}+1}\mathrm{d}x - \int_{-\infty}^{\log(z)} x^{\nu-1}\left(1-\frac{1}{e^{x-\log(z)}+1}\right)\mathrm{d}x\right\} \\
&= \frac{1}{\Gamma(\nu)}\left\{\frac{(\log(z))^\nu}{\nu} + \int_0^\infty \frac{(x+\log(z))^{\nu-1}}{e^x+1}\mathrm{d}x - \int_\infty^0 (\log(z)-x)^{\nu-1}\left(1-\frac{1}{e^{-x}+1}\right)(-\mathrm{d}x)\right\} \\
&= \frac{1}{\Gamma(\nu)}\left\{\frac{(\log(z))^\nu}{\nu} + \int_0^\infty \frac{(x+\log(z))^{\nu-1}-(\log(z)-x)^{\nu-1}}{e^x+1}\mathrm{d}x\right\} \\
&= \frac{1}{\Gamma(\nu)}\left\{\frac{(\log(z))^\nu}{\nu} + \int_0^\infty (\log(z))^{\nu-1}\left(\left(1+\frac{x}{\log(z)}\right)^{\nu-1} - \left(1-\frac{x}{\log(z)}\right)^{\nu-1}\right)\frac{1}{e^x+1}\mathrm{d}x\right\} \\
&= \frac{1}{\Gamma(\nu)}\frac{(\log(z))^\nu}{\nu}\left\{1+\int_0^\infty (\log(\nu))^{-1}\nu\left[\sum_{k=0}^\infty \frac{\Gamma(\nu)}{\Gamma(\nu-k)\Gamma(k+1)}\left(\left(\frac{x}{\log(z)}\right)^k - \left(\frac{-x}{\log(z)}\right)^k\right)\right]\frac{1}{e^x+1}\mathrm{d}x\right\} \\
&= \frac{(\log(\nu))^\nu}{\Gamma(\nu+1)}\left\{1+\int_0^\infty (\log(\nu))^{-1}\nu\left[\sum_{k=0}^\infty \frac{\Gamma(\nu)}{\Gamma(\nu-(2k+1))\Gamma((2k+1)+1)}2\left(\frac{x}{\log(z)}\right)^{2k+1}\right]\frac{1}{e^x+1}\mathrm{d}x\right\} \\
&= \frac{(\log(\nu))^\nu}{\Gamma(\nu+1)}\left\{1+\int_0^\infty (\log(\nu))^{-1}\sum_{k=1}^\infty \frac{\Gamma(\nu+1)}{\Gamma(\nu-(2k-1))\Gamma((2k-1)+1)}\frac{2}{(\log(z))^{2k-1}}\int_0^\infty \frac{x^{2k-1}}{e^x+1}\mathrm{d}x\right\} \\
&= \frac{(\log(\nu))^\nu}{\Gamma(\nu+1)}\left\{1+\sum_{k=1}^\infty \frac{\Gamma(\nu+1)}{\Gamma(\nu-2k+1)\Gamma(2k)}\frac{2}{(\log(z))^{2k}}\left(2^{2k}-2\right)(-1)^{k+1}\frac{\pi^{2k}B_{2k}}{4k}\right\} \\
&= \frac{(\log(\nu))^\nu}{\Gamma(\nu+1)}\left\{1+\sum_{k=1}^\infty \frac{\Gamma(\nu+1)}{\Gamma(\nu-2k+1)\Gamma(2k)}\frac{(2^{2k-1}-1)}{(\log(z))^{2k}}(-1)^{k+1}\frac{\pi^{2k}B_{2k}}{k}\right\} = F_{\nu-1}(\log(z)) \qquad (41)
\end{aligned}
$$

Going back to chemical potential we have **Sommerfeld's lemma**. Here it reads:

$$
\begin{aligned}
f_\nu\left(e^{\beta\mu}\right) &\approx \frac{(\beta\mu)^\nu}{\Gamma(\nu+1)}\left(1+\nu(\nu-1)\frac{\pi^2}{6}(\beta\mu)^{-2}+\nu(\nu-1)(\nu-2)(\nu-3)\frac{7\pi^4}{360}(\beta\mu)^{-4}+\dots\right) \\
&= \frac{(\beta\mu)^\nu}{\Gamma(\nu+1)}\left(1+\sum_{k=1}^\infty \frac{\Gamma(\nu+1)(2^{2k-1}-1)}{\Gamma(\nu-2k+1)\Gamma(2k)}(\beta\mu)^{-2k}(-1)^{k+1}\frac{\pi^{2k}B_{2k}}{k}\right) \approx F_{\nu-1}(\beta\mu) \qquad (42)
\end{aligned}
$$

Similarly now, as is done in Reference [11], one can now also compute quantities like the internal energy in terms of fermi functions. For example we have

$$
U = \frac{\int_0^\infty D(\epsilon)g(\epsilon)\epsilon\mathrm{d}\epsilon}{\int_0^\infty D(\epsilon)g(\epsilon)\mathrm{d}\epsilon} = Nk_BT\frac{\int_0^\infty \frac{x^{3/2}}{z^{-1}e^x+1}\mathrm{d}x}{\int_0^\infty \frac{x^{1/2}}{z^{-1}e^x+1}\mathrm{d}x} = Nk_BT\frac{\Gamma(5/2)}{\Gamma(3/2)}\frac{f_{5/2}(z)}{f_{3/2}(z)} \qquad (43)
$$

Summarizing, in this view we found:

$$
f_\nu\left(e^{\beta\mu}\right) \approx \begin{cases} -\sum_{k=1}^{\mathrm{some}N}\frac{\left(-e^{\beta\mu}\right)^k}{k^\nu} & \text{for } 0<\left(z=e^{\beta\mu}\right)<1 \\ \frac{(\beta\mu)^\nu}{\Gamma(\nu+1)}\left(1+\sum_{k=1}^\infty \frac{\Gamma(\nu+1)(2^{2k-1}-1)}{\Gamma(\nu-2k+1)\Gamma(2k)}(\beta\mu)^{-2k}(-1)^{k+1}\frac{\pi^{2k}B_{2k}}{k}\right) & \text{for large } \left(z=e^{\beta\mu}\right)>>1 \end{cases}
$$

2 The Bernoulli Numbers B_n

2.1 The Generating Function

By generating function usually a function is meant, whose Taylor expansion yields the seeked for expression. In our case it will be a simple fraction:

$$f(x) = \frac{x}{e^x - 1} \quad \forall x \neq 0, \quad f^n(0) = 0, \quad \forall n = 0, 1, \ldots, \quad n \in \mathbb{N}, \tag{44}$$

The Bernoulli numbers are defined to be the coefficients of the taylor expansion for this function. However, to obtain them we have to go a different way than usually.

$$f(x) := \sum_{n=0}^{\infty} \frac{B_n}{n!} x^n \tag{45}$$

by definition we have the taylor series for the exponential function:

$$e^x := \sum_{k=0}^{\infty} \frac{x^k}{k!} \tag{46}$$

$$\begin{aligned} f(x) &= \frac{1}{\left(\sum_{k=0}^{\infty} \frac{x^k}{k!} - 1\right) \frac{1}{x}} = \left(\sum_{k=1}^{\infty} \left(\frac{x^k}{k!}\right) \frac{1}{x}\right)^{-1} = \left(\sum_{k=1}^{\infty} \left(\frac{x^{k-1}}{k!}\right)\right)^{-1} = \left(\sum_{k=0}^{\infty} \left(\frac{x^k}{(k+1)!}\right)\right)^{-1} && (47) \\ &= \sum_{n=0}^{\infty} \frac{B_n}{n!} x^n && (48) \end{aligned}$$

$$\Rightarrow \quad \left(\sum_{n=0}^{\infty} \frac{B_n}{n!} x^n\right) \left(\sum_{k=0}^{\infty} \left(\frac{x^k}{(k+1)!}\right)\right) = 1 \tag{49}$$

Now we make use of the Cauchy Product of series (see Appendix A):

$$1 = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} \frac{B_k x^k}{k!} \frac{x^{n-k}}{(n-k+1)!}\right) = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} B_k \frac{x^n}{k!(n+1-k)!}\right) \tag{50}$$

We use the definition of n choose k to rewrite this (see Appendix B):

$$1 = \sum_{n=0}^{\infty} \left(\sum_{k=0}^{n} B_k \binom{n+1}{k}\right) \frac{x^n}{(n+1)!} \tag{51}$$

This equation is somewhat equivalent to a binomial expression if one defines the exponent of B to be understood as a subscript (Then compare eqn. (51) with (50)):

$$\begin{aligned} (B+1)^{n+1} - B^{n+1} &= \sum_{k=0}^{n+1} B^k 1^{n+1-k} \binom{n+1}{k} - B^{n+1} && (52) \\ &= \sum_{k=0}^{n} B^k \binom{n+1}{k} + B^{n+1} \binom{n+1}{n+1} - B^{n+1} = \sum_{k=0}^{n} B^k \binom{n+1}{k} && (53) \end{aligned}$$

2.2 The Recurrence Formula

Now the procedure of comparison of coefficients yields the first Bernoulli number B_0:

$$1 = \sum_{k=0}^{0} B_k \binom{0+1}{k} \frac{x^0}{(0+1)!} = B_0 \frac{1!}{0!1!} \frac{1!}{1!} \quad \Rightarrow B_0 = 1 \tag{54}$$

For the following numbers we use a **recurrence formula** by noting that comparison of coefficients tells us: For all n greater 0, the sum in the brackets of equation (51) has to vanish!

$$\sum_{k=0}^{n} B_k \binom{n+1}{k} = 0 \quad \forall\, n \geq 1, \quad n \in \mathbb{N}, \tag{55}$$

A nice interpretation of this formula is sugested by the similarity to the Binomial expansion introduced in equation (50) and (51). We only have to write down the appropriate row of the Pascal Triangle for $(B+1)^{n+1}$ without the last term

$$\begin{array}{lcl}
n=1 & 0 = B_0 + B_1 & \Rightarrow B_1 = -\frac{1}{2} \\
n=2 & 0 = B_0 + 3B_1 + 3B_2 & \Rightarrow B_2 = \frac{1}{6} \\
n=3 & 0 = B_0 + 4B_1 + 6B_2 + 4B_3 & \Rightarrow B_3 = 0 \\
n=4 & 0 = B_0 + 5B_1 + 10B_2 + 10B_3 + 5B_4 & \Rightarrow B_4 = -\frac{1}{30} \\
n=5 & 0 = B_0 + 6B_1 + 15B_2 + 20B_3 + 15B_4 + 6B_5 & \Rightarrow B_5 = 0 \\
n=6 & 0 = B_0 + 7B_1 + 21B_2 + 35B_3 + 35B_4 + 21B_5 + 7B_6 & \Rightarrow B_6 = \frac{1}{42}
\end{array}$$

n	0	1	2	4	6	8	10	12	14	16	18	20
B_n	1	$-\frac{1}{2}$	$\frac{1}{6}$	$-\frac{1}{30}$	$\frac{1}{42}$	$-\frac{1}{30}$	$\frac{5}{66}$	$-\frac{691}{2730}$	$\frac{7}{6}$	$-\frac{3617}{510}$	$\frac{43867}{798}$	$-\frac{174611}{330}$

Table 1: some Bernoulli Numbers, note: $B_{2n+1} = 0 \quad \forall n \geq 1$

3 The Riemann-Zeta Function $\zeta(x)$

The aim will be to express the Riemann Zeta function with the help of the Bernoulli numbers. To do so we will find two notions of one and the same expression and eventually compare both to obtain the result.

3.1 First Notion of $\frac{x}{2} \coth \frac{x}{2}$

$$\frac{x}{2}\coth\frac{x}{2} = \frac{x}{2}\frac{\cosh\frac{x}{2}}{\sinh\frac{x}{2}} = \frac{x}{2}\frac{e^{\frac{x}{2}} + e^{-\frac{x}{2}}}{e^{\frac{x}{2}} - e^{-\frac{x}{2}}} \times \overbrace{\frac{e^{\frac{x}{2}}}{e^{\frac{x}{2}}}}^{=1} \tag{56}$$

$$= \frac{x}{2}\frac{e^x + 1}{e^x - 1} = \frac{x}{e^x - 1} + \frac{x}{2} = \sum_{n=0}^{\infty} \frac{B_n}{n!} x^n + \frac{x}{2} \tag{57}$$

If we now note that $B_0 = 1$ and $B_1 = -1/2$ we get

$$\frac{x}{2}\coth\frac{x}{2} = \frac{1x^0}{0!} - \frac{x^1}{2 \times 1!} + \sum_{n=2}^{\infty} \frac{B_n}{n!} x^n + \frac{x}{2} = 1 + \sum_{n=2}^{\infty} \frac{B_n}{n!} x^n \tag{58}$$

Now it also gets clear why table 1 only lists even subscripts of Bernoulli numbers. The cotangens hyperbolicus, being a quotient of an even and an odd function, is odd again. x is an odd function as well, and hence $\frac{x}{2}\coth\frac{x}{2}$ is an even function. Therefore, by this representation of our series we note that $B_{2n+1} = 0$ for all n greater or equal 1. ($B_{2n+1} = 0 \quad \forall n = 1, 2, \ldots$)
Therefore we can write down more succintly:

$$\frac{x}{2}\coth\frac{x}{2} = 1 + \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} x^{2n} \tag{59}$$

3.2 Second Notion of $\frac{x}{2}\coth\frac{x}{2}$

3.2.1 Fourier Series of $\cos(yx)$

In this section we will calculate the Fourier Series of the following function g(x). Later we will take a special value for x in the found expression to continue:

$$g(x) = cos\,(yx)\,, \quad y \in \mathbb{R}\backslash\mathbb{Z}, \quad \mathbb{D} = [-\pi, \pi] \tag{60}$$

The general formula of the Fourier series is:

$$g(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty}(a_k \cos kx + b_k \sin kx) \tag{61}$$

Where it saves a lot of time to note that the coefficients b_k are all zero, since our founction is even! I will also use the following relations during the calculation of a_k:

$$\cos x \cos y = \frac{1}{2}\left[\cos(x-y)\cos(x+y)\right], \qquad \sin(-x) = -\sin(x)$$

$$\sin(a+b) = \sin(a)\cos(b) + \cos(a)\sin(b), \quad \sin(k\pi) = 0, \quad \cos(k\pi) = (-1)^k$$

$$\begin{aligned}
a_k &= \frac{1}{\pi}\int_{-\pi}^{+\pi}\cos yx \cos kx \mathrm{d}x = \frac{1}{\pi}\int_{-\pi}^{+\pi}\frac{1}{2}\left(\cos(yx-kx)\cos(yx+kx)\right)\mathrm{d}x && (62)\\
&= \frac{1}{2\pi}\left[\frac{\sin((y-k)x)}{y-k} + \frac{\cos((y+k)x)}{y+k}\right]_{-\pi}^{\pi} = \frac{1}{\pi}\left(\frac{\sin((y-k)\pi)}{y-k} + \frac{\cos((y+k)\pi)}{y+k}\right) && (63)\\
&= \frac{1}{\pi}\left(\frac{(y+k)\left(\sin y\pi\cos k\pi - \sin k\pi\cos y\pi\right) + (y-k)\left(\sin y\pi cos k\pi + \sin k\pi\cos y\pi\right)}{(y+k)(y-k)}\right) && (64)\\
&= \frac{1}{\pi}\left(\frac{y\sin(y\pi)(-1)^k + k\sin(y\pi)(-1)^k + y\sin(y\pi)(-1)^k - k\sin(y\pi)(-1)^k}{y^2-k^2}\right) && (65)\\
&= \frac{1}{\pi}\left(\frac{2y\sin(y\pi)(-1)^k}{y^2-k^2}\right) && (66)
\end{aligned}$$

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{+\pi}\cos(yx)\mathrm{d}x = \frac{1}{\pi}\left[\frac{1}{y}\sin(yx)\right]_{-\pi}^{+\pi} = \frac{1}{\pi}\left(\frac{2}{y}\sin(y\pi)\right) \tag{67}$$

Plugging these coefficients back into equation (61) gives our Fourier Series of g(x):

$$\cos(yx) = \frac{\sin(y\pi)}{y\pi} + \sum_{k=1}^{\infty}\frac{1}{\pi}\left(\frac{2y\sin(y\pi)(-1)^k}{y^2-k^2}\right)\cos(kx) \tag{68}$$

Now we consider the special case $x = \pi$:

$$\cos(y\pi) = \frac{\sin(y\pi)}{\pi}\left[\frac{1}{y} + \sum_{k=1}^{\infty}\left(\frac{2y(-1)^k}{y^2-k^2}\right)(-1)^k\right] \tag{69}$$

$$\Rightarrow \pi \times \frac{\cos(y\pi)}{\sin(y\pi)} = \frac{1}{y} + \sum_{k=1}^{\infty}\frac{2y}{y^2-k^2} = \pi\cot(y\pi) \tag{70}$$

This is the so-called **partial fraction decomposition** of the cotangens function.

3.2.2 Transformation to $\frac{x}{2}\coth\frac{x}{2}$

We will now transform the regular cotangens and its partial fraction decomposition into the second form of the cotangens hyperbolicus we need for the comparison ahead.

$$\cot(iy') = \frac{\frac{1}{2}\left(e^{i\times iy'}+e^{-i\times iy'}\right)}{\frac{1}{2i}\left(e^{i\times iy'}-e^{-i\times iy'}\right)} = i\,\frac{\left(e^{-y'}+e^{y'}\right)}{\left(e^{-y'}-e^{y'}\right)} = -i\coth(y') \tag{71}$$

We multiply this equation by $i\pi$ and let $y' = y\pi$ to fit our purposes:

$$i\pi\cot(iy') = \pi\coth(y') \Rightarrow i\pi\cot(iy\pi) = \pi\coth(y\pi) \tag{72}$$

$$\pi\coth(y\pi) = i\left[\frac{1}{iy}+\sum_{k=1}^{\infty}\frac{2iy}{(iy)^2-k^2}\right] = \frac{1}{y}+\sum_{k=1}^{\infty}\frac{-2y}{-y^2-k^2} = \frac{1}{y}+\sum_{k=1}^{\infty}\frac{2y}{y^2+k^2} \tag{73}$$

Now we will do the following substitution to get the right arguement in the cotangens hyperbolicus:

$$y\pi = \frac{x}{2} \quad\Rightarrow\quad y = \frac{x}{2\pi} \quad\Rightarrow\quad \pi = \frac{x}{2y} \tag{74}$$

$$\frac{x}{2y}\coth\left(\frac{x}{2}\right) = \frac{1}{y}+\sum_{n=1}^{\infty}\frac{2y}{\frac{x^2}{4\pi^2}+n^2} \tag{75}$$

$$\Rightarrow \frac{x}{2}\coth\left(\frac{x}{2}\right) = 1+\sum_{n=1}^{\infty}\frac{2\frac{x^2}{4\pi^2}}{\frac{x^2}{4\pi^2}+n^2} = 1+\sum_{n=1}^{\infty}\frac{2x^2}{x^2+4\pi^2n^2} \tag{76}$$

We need to recognize that this infinite sum represents a geometric series (see Appendix C)

$$-\sum_{k=1}^{\infty}\left(-\frac{x^2}{4\pi^2n^2}\right)^k = -\frac{-\frac{x^2}{4\pi^2n^2}}{1+\frac{x^2}{4\pi^2n^2}} = \frac{x^2}{x^2+4\pi^2n^2} \tag{77}$$

$$= \sum_{k=1}^{\infty}(-1)^{k+1}\left(\frac{x}{2\pi n}\right)^{2k} \tag{78}$$

$$\Rightarrow \frac{x}{2}\coth\left(\frac{x}{2}\right) = 1+2\sum_{n=1}^{\infty}\sum_{k=1}^{\infty}(-1)^{k+1}\left(\frac{x}{2\pi n}\right)^{2k} = 1+2\sum_{k=1}^{\infty}\left[(-1)^{k+1}\sum_{n=1}^{\infty}\frac{1}{(2\pi n)^{2k}}\right]x^{2k} \tag{79}$$

3.3 Comparison and Result

Now we compare our found equations (79) and (59)

$$\frac{x}{2}\coth\left(\frac{x}{2}\right) = 1+2\sum_{k=1}^{\infty}\left[(-1)^{k+1}\sum_{n=1}^{\infty}\frac{1}{(2\pi n)^{2k}}\right]x^{2k} \tag{80}$$

$$= 1+\sum_{n=1}^{\infty}\frac{B_{2n}}{(2n)!}x^{2n} \tag{81}$$

$$\Rightarrow \sum_{k=1}^{\infty}\left[(-1)^{k+1}\sum_{n=1}^{\infty}\frac{1}{(2\pi n)^{2k}}\right]x^{2k} = \frac{1}{2}\sum_{k=1}^{\infty}\frac{B_{2k}}{(2k)!}x^{2k} \tag{82}$$

Comparison of coefficients yields:

$$(-1)^{k+1}\sum_{n=1}^{\infty}\frac{1}{(2\pi n)^{2k}} = \frac{1}{2}\frac{B_{2k}}{(2k)!} \tag{83}$$

$$\sum_{n=1}^{\infty}\frac{1}{n^{2k}} = (-1)^{k+1}(2\pi)^{2k}\frac{B_{2k}}{2(2k)!} = \zeta(2k) \tag{84}$$

This is the final result for the **Riemann Zeta function of even integers**. Up to now, there is no closed form for odd integers known to man. It also follows (since we have a sum of non negative numbers) that $B_{2k}(-1)^{k+1} \geq 0$.

3.4 Application

The first few results of the Riemann Zeta function are the following:

$$\underbrace{\zeta(2)}_{k=1} = \sum_{n=1}^{\infty}\frac{1}{n^2} = (-1)^2(2\pi)^2\frac{B_2}{2(2)!} = \pi^2 B_2 = \frac{\pi^2}{6} \tag{85}$$

$$\underbrace{\zeta(4)}_{k=2} = \sum_{n=1}^{\infty}\frac{1}{n^4} = (-1)^3(2\pi)^4\frac{B_4}{2(4)!} = -\frac{2^3\pi^4}{4!}B_4 = \frac{\pi^4}{90} \tag{86}$$

$$\underbrace{\zeta(6)}_{k=3} = \sum_{n=1}^{\infty}\frac{1}{n^6} = (-1)^4(2\pi)^6\frac{B_6}{2(6)!} = \frac{2^6\pi^6}{2\times 6!}B_6 = \frac{\pi^6}{945} \tag{87}$$

Further studies on and special application of the Riemann Zeta function:

$$\underbrace{\sum_{n=0}^{\infty}\frac{1}{(2n+2)^p}}_{\text{even numbers}} = \frac{1}{2^p}\left(\frac{1}{1^p}+\frac{1}{2^p}+\frac{1}{3^p}+\frac{1}{4^p}+\dots\right) = \frac{1}{(1\times 2)^p}+\frac{1}{(2\times 2)^p}+\frac{1}{(3\times 2)^p}+\frac{1}{(4\times 2)^p}+\dots \tag{88}$$

$$= \frac{1}{2^p}+\frac{1}{4^p}+\frac{1}{6^p}+\frac{1}{8^p}+\dots = \frac{1}{2^p}\sum_{n=1}^{\infty}\frac{1}{n^p} = \frac{1}{2^p}\zeta(p) \tag{89}$$

$$\zeta(p) = \sum_{n=1}^{\infty}\frac{1}{n^p} = \underbrace{\sum_{n=0}^{\infty}\frac{1}{(2n+1)^p}}_{\text{odd numbers}} + \underbrace{\sum_{n=0}^{\infty}\frac{1}{(2n+2)^p}}_{\text{even numbers}} = \sum_{n=0}^{\infty}\frac{1}{(2n+1)^p} + \frac{1}{2^p}\sum_{n=1}^{\infty}\frac{1}{n^p} \tag{90}$$

$$\Rightarrow \quad \zeta(p) - \frac{1}{2^p}\zeta(p) = \sum_{n=0}^{\infty}\frac{1}{(2n+1)^p} = \frac{2^p-1}{2^p}\zeta(p) \tag{91}$$

$$\frac{1}{1^p}-\frac{1}{2^p}+\frac{1}{3^p}-\frac{1}{4^p}+\frac{1}{5^p} = 2\sum_{n=0}^{\infty}\frac{1}{(2n+1)^p} - \sum_{n=0}^{\infty}\frac{1}{(n+1)^p} = \left(2\left(\frac{2^p-1}{2^p}\right)-1\right)\zeta(p) \tag{92}$$

$$= \left(\frac{2^p-2}{2^p}\right)\zeta(p) = \sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)^p} \tag{93}$$

Summarizing we have also found the following infinite series:

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)^p} = \frac{2^p-2}{2^p}\zeta(p) \tag{94}$$

$$\sum_{n=0}^{\infty}\frac{1}{(2n+1)^p} = \frac{2^p-1}{2^p}\zeta(p) \tag{95}$$

$$\sum_{n=0}^{\infty}\frac{1}{(2n+2)^p} = \frac{1}{2^p}\zeta(p) \tag{96}$$

Note that one can not put $p=1$ in equation (94) to obtain a result for $\zeta(1)$ in dependnece on $\ln(2)$ since the Riemann zeta function has a singularity at this point due to its reduction to the diverging harmonic series there.

APPENDIX

A Cauchy Product

$$\left(\sum_{n=0}^{\infty} a_n\right)\left(\sum_{n=0}^{\infty} b_n\right) = \sum_{n=0}^{\infty}\left(\sum_{k=0}^{n} a_k b_{n-k}\right) \tag{97}$$

Note: If both series on the left converge absolutely, the Cauchy series converges absolutely as well. In this case, its limit is the product of the limits of the series on the left.

B n choose k

$$\binom{n}{k} := \frac{n!}{k!(n-k)!} \qquad \text{for } n,k \in \mathbb{N} \tag{98}$$

C The Geometric Series

$$s_n = 1 + q^1 + q^2 + q^3 + \ldots + q^n \tag{99}$$

$$s_n \times q = q + q^2 + q^3 + \ldots + q^n + q^{n+1} \tag{100}$$

Substraction of equation (112) from (111) gives

$$s_n(1-q) = 1 - q^{n+1} \quad \Rightarrow \quad s_n = \sum_{k=0}^{n} q^k = \frac{1-q^{n+1}}{1-q} \tag{101}$$

$$s_n - s_{n_0} = \sum_{k=n_0}^{n} q^k = \frac{1-q^{n+1}}{1-q} - \frac{1-q^{n_0-1+1}}{1-q} = \frac{q^{n_0}-q^{n+1}}{1-q} \quad \Rightarrow \quad \sum_{k=n_0}^{\infty} q^k = \frac{q^{n_0}}{1-q} \text{ for } \left|q\right| \leq 1 \tag{102}$$

$$\Rightarrow \quad \sum_{k=1}^{\infty} z^k = \frac{z}{1-z} \tag{103}$$

D Special Functions

$$\left(\frac{1}{2\cosh(z/2)}\right)^2 = \left(\frac{1}{\left(e^{z/2}+e^{-z/2}\right)}\frac{e^{z/2}}{e^{z/2}}\right)^2 = \frac{e^z}{(e^z+1)^2} \tag{104}$$

$$\Gamma(x) = \int_0^{\infty} z^{x-1} e^{-z} \mathrm{d}z = (x-1)\Gamma(x-1) = (x-1)! \quad \text{for } x \in \mathbb{N} \tag{105}$$

$$\zeta(x) = \sum_{n=1}^{\infty} \frac{1}{n^x} \tag{106}$$

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