Sommerfeld functional equation

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Abstract

We derive the well-known Sommerfeld expansion of the Fermi-Dirac integral, and then deduce a functional equation for the chemical potential which we denote here by $h(y)$ where y is the absolute temperature in energy units.

1 First property definitions

Let a real function F of the real variable y be given, with integral representation:

$$F(y) = \int_0^{+\infty} K(\xi, y)\, d\xi, \quad \forall y \in (0, +\infty) \tag{1}$$

The kernel $K(\xi, y)$ is

$$K(\xi, y) = \frac{f(\xi)}{e^{\frac{\xi - h(y)}{y}} + 1} \tag{2}$$

where: 1) $f \in C^{\omega}(0, +\infty)$ is there positive and such that the integral (1) is convergent; 2) $h(y) \in C^1(0, +\infty)$ and positive there.

Proposition 1 *$y = 0$ is a eliminating point of discontinuity forf (y).*

Proof. Let's calculate

$$\lim_{y \to 0^+} F(y) = \int_0^{+\infty} \lim_{y \to 0^+} K(\xi, y)\, d\xi$$

Let's determine separately:

$$\lim_{y \to 0^+} K(\xi, y) = \frac{f(\xi)}{1 + \lim_{y \to 0^+} e^{\frac{\xi - h(y)}{y}}}$$

But

$$\lim_{y \to 0^+} e^{\frac{\xi - h(y)}{y}} = \begin{cases} e^{-\infty} = 0^+, & 0 \leq \xi < h(0) \\ e^{+\infty}, & \xi > h(0) \end{cases}$$

so

$$\lim_{y \to 0^+} K(\xi, y) = \begin{cases} \frac{f(\xi)}{1 + 0^+} = f(\xi), & 0 \leq \xi < h(0) \\ \frac{f(\xi)}{1 + (+\infty)} = 0^+, & \xi > h(0) \end{cases}$$

$$\Longrightarrow \lim_{y \to 0^+} F(y) = \int_0^{h(0)} f(\xi)\, d\xi$$

hence the statement ■

From this proposition it follows that we can prolong by continuity $F(y)$:

$$F(y) = \begin{cases} \int_0^{+\infty} \frac{f(\xi) d\xi}{e^{\frac{\xi - h(y)}{y}} + 1}, & y > 0 \\ \int_0^{h(0)} f(\xi)\, d\xi, & y = 0 \end{cases} \tag{3}$$

2 Sommerfeld expansion

Lemma 2 *For each* $\lambda > 0$

$$\int_0^{+\infty} \frac{t^\lambda}{e^t+1} dt = \left(1-2^{1-\lambda}\right) \Gamma(\lambda) \zeta(\lambda), \qquad k = 1, 2, ... \tag{4}$$

where $\Gamma(\lambda)$ *and* $\zeta(\lambda)$ *are respectively the gamma function [1] and the Zeta Riemann function [2].*

Proof. We write

$$\frac{1}{e^t+1} = \frac{e^{-t}}{1+e^{-t}} = e^{-t} \sum_{n=0}^{+\infty} (-1)^n e^{-(nt)}$$

The last step is justified by the position $\tau = e^{-t} < 1$ for $t > 0$, so

$$\frac{1}{1+\tau} = \sum_{n=0}^{+\infty} (-1)^n \tau^n$$

It follows

$$\begin{aligned} \int_0^{+\infty} \frac{t^{\lambda-1} dt}{e^t+1} &= \int_0^{+\infty} t^{\lambda-1} e^{-t} \sum_{n=0}^{+\infty} (-1)^n e^{-(nt)} dt \\ &= \sum_{n=0}^{+\infty} (-1)^n \int_0^{+\infty} t^{\lambda-1} e^{-(n+1)t} dt \\ &\underset{\eta=(n+1)t}{=} \sum_{n=0}^{+\infty} (-1)^n \frac{1}{(n+1)^\lambda} \underbrace{\int_0^{+\infty} \eta^{\lambda-1} e^{-\eta} d\eta}_{\Gamma(\lambda)} \end{aligned}$$

while in the other term we recognize the alternating series

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

Hence the statement. ■

Theorem 3 *(***Sviluppo di Sommerfeld***)*
The following asymptotic evolution exists:

$$y \ll h(0) \Longrightarrow F(y) = \int_0^{h(y)} f(\xi) d\xi + 2y \sum_{k=1}^{+\infty} c_k y^{2k-1} f^{(2k-1)}(h(y)) \tag{5}$$

where

$$c_k = \left(1-2^{1-2k}\right) \zeta(2k) \tag{6}$$

Proof. Let's say

$$x = \frac{\xi - h(y)}{y} \Longrightarrow d\xi = y dx, \quad -\frac{h(y)}{y} \le x < +\infty$$

Continued

$$F\left(y\right)=y\int_{-\frac{h(y)}{y}}^{+\infty}\frac{f\left(h\left(y\right)+yx\right)dx}{e^{x}+1}=\underbrace{y\int_{-\frac{h(y)}{y}}^{0}\frac{f\left(h\left(y\right)+yx\right)dx}{e^{x}+1}}_{I_{1}(y)}+y\int_{0}^{+\infty}\frac{f\left(h\left(y\right)+yx\right)dx}{e^{x}+1} \tag{7}$$

Let's calculate separately

$$I_{1}\left(y\right)=\int_{-\frac{h(y)}{y}}^{0}\frac{f\left(h\left(y\right)+yx\right)dx}{e^{x}+1} \tag{8}$$

Let's perform the change of variable:

$$x'=-x\Longrightarrow dx=-dx',\quad -\frac{h\left(y\right)}{y}\leq x=-x'\leq 0\Longrightarrow\frac{h\left(y\right)}{y}\geq x'\geq 0$$

So

$$I_{1}\left(\ y\right)=-\int_{\frac{h(y)}{y}}^{0}\frac{f\left(h\left(y\right)-yx'\right)dx'}{e^{-x'}+1}=\int_{0}^{\frac{h(y)}{y}}\frac{f\left(h\left(y\right)-yx'\right)dx'}{e^{-x'}+1}\underset{x'=\text{variabile muta}}{=}\int_{0}^{\frac{h(y)}{y}}\frac{f\left(h\left(y\right)-yx\right)dx}{e^{-x}+1} \tag{9}$$

Furthermore

$$\frac{1}{e^{-x}+1}=\frac{1}{e^{-x}\left(1+e^{x}\right)}=\frac{e^{x}}{1+e^{x}}=\frac{e^{x}+1-1}{e^{x}+1}=1-\frac{1}{e^{x}+1},$$

i.e.

$$I_{1}\left(y\right)=\int_{0}^{\frac{h(y)}{y}}\frac{f\left(h\left(y\right)-yx\right)dx}{e^{-x}+1}=\underbrace{\int_{0}^{\frac{h(y)}{y}}f\left(h\left(y\right)-yx\right)dx}_{I_{2}(y)}-\int_{0}^{\frac{h(y)}{y}}\frac{f\left(h\left(y\right)-yx\right)dx}{e^{x}+1} \tag{10}$$

In the integral $I_{2}\left(y\right)$ we perform the change of variable:

$$x'=-x\Longrightarrow I_{2}\left(y\right)=\int_{-\frac{h(y)}{y}}^{0}f\left(h\left(y\right)-yx'\right)dx'=\int_{-\frac{h(y)}{y}}^{0}f\left(h\left(y\right)-yx\right)dx \tag{11}$$

Resetting the variable $\xi=h\left(y\right)+yx$

$$dx=\frac{1}{y}d\xi,\quad -\frac{h\left(y\right)}{y}\leq x=\frac{\xi-h\left(y\right)}{y}\leq 0\Longrightarrow 0\leq\xi\leq h\left(y\right)$$

i.e.

$$I_{2}\left(y\right)=\frac{1}{y}\int_{0}^{\mu(y)}f\left(\xi\right)d\xi \tag{12}$$

Substituting the various expressions:

$$I_{1}\left(y\right)=\frac{1}{y}\int_{0}^{h(y)}f\left(\xi\right)d\xi-\int_{0}^{\frac{h(y)}{y}}\frac{f\left(h\left(y\right)-yx\right)dx}{e^{x}+1} \tag{13}$$

So

$$\int_{0}^{+\infty}\frac{f\left(\xi\right)d\xi}{e^{\frac{\xi-h(y)}{y}}+1}=\int_{0}^{h(y)}f\left(\xi\right)d\xi+y\int_{0}^{+\infty}\frac{f\left(h\left(y\right)+yx\right)dx}{e^{x}+1}-y\int_{0}^{\frac{h(y)}{y}}\frac{f\left(h\left(y\right)-yx\right)dx}{e^{x}+1} \tag{14}$$

We have thus broken the integral on the first member into the sum of three contributions, two of which are ordinary integrals. In (14) we focus on the integra

$$\int_0^{\frac{h(y)}{y}} \frac{f\left(h\left(y\right)-yx\right)dx}{e^x+1} \underset{y\ll h(y)}{\longrightarrow} \int_0^{+\infty} \frac{f\left(h\left(y\right)-yx\right)dx}{e^x+1} \tag{15}$$

It follows

$$F\left(y \ll h\left(0\right)\right) = \int_0^{h(y)} f\left(\xi\right)d\xi + y\left[\int_0^{+\infty} \frac{f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right)}{e^x+1}dx\right] \tag{16}$$

The hypothesis of the analyticity of the function f allows us to develop $f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right)$ in Taylor series according to the powers of x:

$$f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right) = \sum_{k=0}^{+\infty}\frac{1}{k!}\left[\frac{d^k}{dx^k}\left(f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right)\right)\right]_{x=0} x^k \tag{17}$$

Calculating the derivatives:

$$\frac{d^k}{dx^k}\left(f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right)\right) = y^k\left[f^{(k)}\left(h\left(y\right)+yx\right)-\left(-1\right)^k f^{(k)}\left(h\left(y\right)-yx\right)\right]$$

so that

$$\left[\frac{d^k}{dx^k}\left(f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right)\right)\right]_{x=0} = \begin{cases} 2y^k y^{(k)}\left(h\left(y\right)\right), & \text{per } n \text{ dispari} \\ 0, & \text{per } n \text{ pari}\end{cases}$$

(17) is rewritten

$$f\left(h\left(y\right)+yx\right)-f\left(h\left(y\right)-yx\right) = 2\sum_{k=1}^{+\infty}\frac{y^{2k-1}f^{(2k-1)}\left(h\left(y\right)\right)}{(2k-1)!}x^{2k-1} \tag{18}$$

which replaced in (**??**) gives:

$$F\left(y \ll h\left(y\right)\right) = \int_0^{h(y)} f\left(\xi\right)d\xi + 2y\sum_{k=1}^{+\infty}\frac{y^{2k-1}f^{(2k-1)}\left(h\left(y\right)\right)}{(2k-1)!}\int_0^{+\infty}\frac{x^{2k-1}}{e^x+1}dt \tag{19}$$

The statement follows from the lemma (2). ■

3 Sommerfeld functional equation

Let's explain some terms in (5):

$$F\left(y\right) = \int_0^{h(y)} f\left(\xi\right)d\xi + \frac{\pi^2}{6}y^2 f'\left(h\left(y\right)\right) + \frac{7\pi^4}{360}y^4 f'''\left(h\left(y\right)\right) + ...$$

In applications [2] is sufficient to truncate at the end of the second order in y:

$$F\left(y\right) = \int_0^{h(y)} f\left(\xi\right)d\xi + \frac{\pi^2}{6}y^2 f'\left(h\left(y\right)\right) \tag{20}$$

while the function $f(\xi)$ is assigned. It follows that (20) is a functional equation in $h(y)$. The following case is of physical interest:

$$f(\xi) = A\xi^{1/2}$$

with $F(y)$ constant function:

$$F(y) = C > 0, \ \ \forall y \in [0, +\infty)$$

It follows

$$C = F(0) = A\int_0^{h(0)} \xi^{1/2} d\xi = \frac{2A}{3} h(0)^{3/2}$$

so

$$F(y) = \frac{2A}{3} h(0)^{3/2}, \ \ \forall y \in [0, +\infty) \tag{21}$$

Substituting in (20):

$$h(0)^{3/2} = h(y)^{3/2} + \frac{\pi^2}{8}\left[\frac{y}{h(y)}\right]^2$$

which can be rewritten as

$$h(y) = \frac{h(0)}{(1+\eta)^{2/3}} \tag{22}$$

where

$$\eta = \frac{\pi^2}{8}\left[\frac{y}{h(0)}\right]^2$$

having used the approximation $\frac{y}{h(y)} \simeq \frac{y}{h(0)}$since is $y \ll h(0)$. It follows $\eta \ll 1$ so $(1+\eta)^{2/3} \simeq 1 - \frac{2}{3}\eta$, and therefore

$$h(y) \simeq h(0)\left(1 - \frac{2}{3}\eta\right)$$

Finally

$$h(y) \simeq h(0)\left[1 - \frac{\pi^2}{12}\left(\frac{y}{h(0)}\right)^2\right], \quad y \ll h(0)$$

ovvero la soluzione dell'equazione funzionale di Sommerfeld.

References

[1] Smirnov V.I. *Corso di Matematica superiore, vol. II*. Editori Riuniti.

[2] Landau L.D., Lifshitz E.M. *Statistical Physics, Third Edition, Part 1: Volume 5* . Editori Riuniti.