Energy of an ideal Fermi gas and the Riemann Zeta function

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Abstract

The values assumed by the Riemann Zeta function on even natural integers contribute to the calculation of the total energy of an ideal Fermi gas in a non-relativistic and strongly degenerate regime.

The Fermi-Dirac integral

If $\mathbb{R}^+ = [0, +\infty)$, let's consider

$$f: \underset{t \longrightarrow f(t), \ \forall t \in \mathbb{R}^+}{\mathbb{R}^+ \longrightarrow \mathbb{R}^+} \tag{1}$$

Precisely, f is the *Fermi-Dirac function*:

$$f(t, y) = \frac{1}{e^{\frac{t - f_1(y)}{y}} + 1} \tag{2}$$

where $y > 0$ is a parameter, while $f_1 \in C^\omega(\mathbb{R}^+)$ is positive in $\mathbb{R}^+$and not necessarily equipped with an elementary expression.

Let's define the function

$$\Lambda(t) = \lim_{y \to 0^+} f(t, y) \tag{3}$$

If $f_1(0) \overset{def}{=} t_0 > 0$

$$\lim_{y \to 0^+} \frac{t - f_1(y)}{y} = \begin{cases} -\infty, & 0 \le t \le t_0 \\ +\infty, & t > t_0 \\ \frac{0}{0}, & t = t_0 \end{cases}, \tag{4}$$

so

$$\Lambda(t) \equiv f(y, 0) = \begin{cases} \frac{1}{e^{-\infty}+1} = 1^-, & 0 \le t \le t_0 \\ \frac{1}{e^{+\infty}+1} = 0^+, & t > t_0 \end{cases} \tag{5}$$

In Fig. 1 we report the trend of $f(y, 0)$.

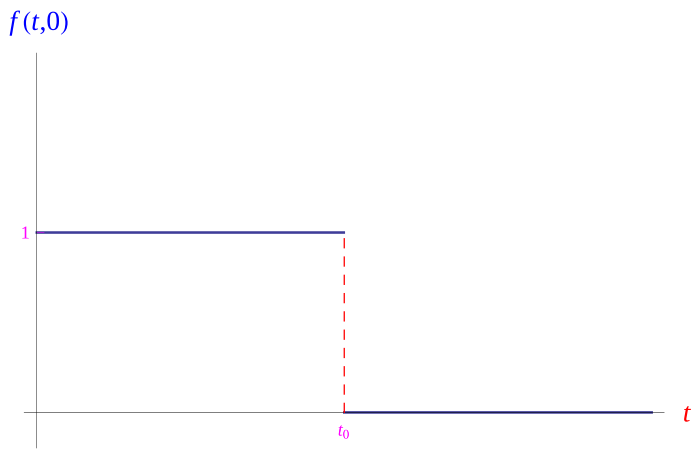

Figure 1: Trend of the Fermi-Dirac function for $y = 0$.

In Quantum Statistical Mechanics (QSM) [1] some quantities are represented by a class of functions that cannot be expressed in elementary terms:

Definition 1 **Fermi-Dirac integral**

$$F_D(y) = \int_0^{+\infty} \varphi(t) f(t,y)\, dt \tag{6}$$

where $f(t,y)$ is the Fermi-Dirac function (2), while $\varphi(t) \geq 0$ is a function with derivatives of a high order and such as to make the integral on the second member of the equation convergent (6).

From (6):

$$F_D(y) = \int_0^{+\infty} \frac{\varphi(t)\, dt}{e^{\frac{t-f_1(y)}{y}} + 1} \tag{7}$$

From the study of the sign of the integrating function in (7) and from known properties of generalized integrals, we have $0 \leq F_D(y) < +\infty$, $\forall y \in \mathbb{R}^+$, where the inequality in the strict sense $< +\infty$ follows from the hypothesis of convergence of the corresponding integral.

Given this, the theorem holds:

Theorem 2 *(***Sommerfeld expansion***)*

For $0 < y \ll f_1(0)$, up to exponentially small terms:

$$F_D(y) = \Phi(f_1(y)) + 2y \sum_{k=1}^{+\infty} u_k(y) \tag{8}$$

where:

$$\Phi(t) = \int_0^t \varphi(t')\, dt' \tag{9}$$

$$u_k(y) = y^{2k-1} \varphi^{(2k-1)}(f_1(y)) \left(1 - 2^{1-2k}\right) \zeta(2k)$$

Here is $\varphi^{(2k-1)}(t) = \frac{d^{2k-1}}{dt^{2k-1}} \varphi(t)$, while ζ is the Riemann zeta function [2].

Dimostrazione. Performing the variable change:

$$x = \frac{t - f_1(y)}{y} \tag{10}$$

The integral (7) becomes:

$$F_D(y) = y \int_{-\frac{f_1(y)}{y}}^{+\infty} \frac{\varphi(f_1(y) + xy)\, dx}{e^x + 1} \tag{11}$$

For the decomposition property:

$$F_D(y) = y \underbrace{\int_{-\frac{f_1(y)}{y}}^{0} \frac{\varphi(f_1(y) + xy)\, dx}{e^x + 1}}_{\stackrel{def}{=} I_1(y)} + y \int_0^{+\infty} \frac{\varphi(f_1(y) + xy)\, dx}{e^x + 1} \tag{12}$$

In $I_1(y)$ we set $x' = -x$

$$I_1(y) = \int_0^{\frac{f_1(y)}{y}} \frac{\varphi(f_1(y) - x'y)\, dx'}{e^{-x'} + 1}$$

Redefining the mute variable x'

$$I_1(y) = \int_0^{\frac{f_1(y)}{y}} \frac{\varphi(f_1(y) - xy)\,dx}{e^{-x} + 1} \tag{13}$$

Furthermore

$$\frac{1}{e^{-x}+1} = 1 - \frac{1}{e^{x}+1}$$

which when replaced (13) returns

$$I_1(y) = I_2(y) - \int_0^{\frac{f_1(y)}{y}} \frac{\varphi(f_1(y) - xy)\,dx}{e^{x} + 1} \tag{14}$$

where

$$I_2(y) \stackrel{def}{=} \int_0^{\frac{f_1(y)}{y}} \varphi(f_1(y) - xy)\,dx \tag{15}$$

If in the integral (15) we set $x' = -x$ and then redefine the integration variable, we obtain:

$$I_2(y) = \int_{-\frac{f_1(y)}{y}}^{0} \varphi(f_1(y) + xy)\,dx \tag{16}$$

Restoring the old variable $t = f_1(y) + xy$ we have:

$$I_2(y) = \frac{1}{y}\int_0^{f_1(y)} \varphi(t)\,dt \tag{17}$$

Replacing (17) in (14):

$$I_1(y) = \frac{1}{y}\int_0^{f_1(y)} \varphi(t)\,dt - \int_0^{\frac{f_1(y)}{y}} \frac{\varphi(f_1(y) - xy)\,dx}{e^{x} + 1} \tag{18}$$

From (12):

$$F_D(y) = yI_1(y) + \int_0^{+\infty} \frac{\varphi(f_1(y) + xy)\,dx}{e^{x} + 1} \tag{19}$$

Replacing (18) in (19):

$$\begin{aligned} F_D(y) = &\int_0^{f_1(y)} \varphi(t)\,dt - y\int_0^{\frac{f_1(y)}{y}} \frac{\varphi(f_1(y) - xy)\,dx}{e^{x} + 1} \\ &+ y\int_0^{+\infty} \frac{\varphi(f_1(y) + xy)\,dx}{e^{x} + 1} \end{aligned} \tag{20}$$

which is an exact expression for $F_D(y)$. In QSM the limit $0 < y \ll f_1(0) = t_0$ is important. Considering $y \ll f_1(y)$ for $0 < y \ll t_0$, in the second integral on the second member of (20) we can place $+\infty$ in the upper limit of integration. This approximation is legitimate thanks to the speed of convergence due to the exponential in the denominator[1]. In that order of approximation:

$$F_D(y) \underset{y \ll f_1(0)}{=} \int_0^{f_1(y)} \varphi(t)\,dt + y\int_0^{+\infty} \frac{\varphi(f_1(y) + xy) - \varphi(f_1(y) - xy)}{e^{x} + 1} dx \tag{21}$$

[1]This is equivalent to neglecting exponentially small terms.

For the hypotheses made on $\varphi(t)$, we can develop $\varphi(f_1(y)+xy)-\varphi(f_1(y)-xy)$ in power series of x and then perform a series integration:

$$\varphi(f_1(y)+xy)-\varphi(f_1(y)-xy)=\sum_{k=0}^{+\infty}\frac{1}{k!}\left[\frac{d^k}{dx^k}(f_1(y)+xy)-\varphi(f_1(y)-xy)\right]_{x=0}x^k$$

Calculating the derivatives

$$\left[\frac{d^k}{dx^k}(f_1(y)+xy)-\varphi(f_1(y)-xy)\right]_{x=0}=\begin{cases}2y^k\varphi^{(k)}(f_1(y)), & \text{per } k \text{ pari}\\ 0, \ \text{per } k \text{ dispari}\end{cases}$$

i.e.

$$\varphi(f_1(y)+xy)-\varphi(f_1(y)-xy)=2\sum_{k=1}^{+\infty}\frac{y^k\varphi^{(k)}(f_1(y))}{(2k-1)!}x^{2k-1}$$

which replaced in (21):

$$F_D(y)\underset{y\ll f_1(0)}{=}\int_0^{f_1(y)}\varphi(t)\,dt+2y\sum_{k=1}^{+\infty}\frac{y^k\varphi^{(k)}(f_1(y))}{(2k-1)!}\int_0^{+\infty}\frac{x^{2k-1}}{e^x+1}dx \tag{22}$$

We therefore have a series of functions whose terms contain the integrals

$$\int_0^{+\infty}\frac{x^{2k-1}}{e^x+1}dx$$

We set

$$J(\sigma)=\int_0^{+\infty}\frac{x^{\sigma-1}}{e^x+1}dx,\quad(\sigma>0) \tag{23}$$

We write

$$\frac{1}{e^x+1}=\frac{e^{-x}}{1+e^{-x}}$$

$(1+e^{-x})^{-1}$ is the sum of a series:

$$\frac{1}{1+e^{-x}}=\sum_{n=0}^{+\infty}(-1)^n e^{-nx}\Longrightarrow\frac{1}{e^x+1}=e^{-x}\sum_{n=0}^{+\infty}(-1)^n e^{-nx}$$

which replaced in (23):

$$J(\sigma)=\sum_{n=0}^{+\infty}(-1)^n e^{-nx}\int_0^{+\infty}x^{\sigma-1}e^{-(n+1)x}dx \tag{24}$$

Performing the change of variable $y=(n+1)x$

$$J(\sigma)=\sum_{n=0}^{+\infty}\frac{(-1)^n}{(n+1)^\sigma}\int_0^{+\infty}y^{\sigma-1}e^{-y}dy \tag{25}$$

The integral is the representation of the Eulerian function gamma for$\sigma>0$:

$$\Gamma(\sigma)=\int_0^{+\infty}y^{\sigma-1}e^{-y}dy$$

The series

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

converges for $\sigma>0$ and its sum is:

$$\sum_{n=1}^{+\infty}\frac{(-1)^n}{n^\sigma}=\left(1-2^{1-\sigma}\right)\zeta\left(\sigma\right)\tag{26}$$

where $\zeta\left(\sigma\right)$ is the Riemann zeta function [2]. In tal modo otteniamo la seguente espressione per $J\left(\sigma\right)$

$$J\left(\sigma\right)=\left(1-2^{1-\sigma}\right)\Gamma\left(\sigma\right)\zeta\left(\sigma\right),\quad\forall\sigma>0\tag{27}$$

In particular

$$\int_0^{+\infty}\frac{x^{2k-1}}{e^x+1}dx=\left(1-2^{1-2k}\right)(2k-1)!\zeta\left(2k\right)\tag{28}$$

because $\Gamma\left(2k\right)=(2k-1)!$. The statement follows from the substitution of (28) in (22). ■

Notation 3 *$\zeta\left(2k\right)$ is expressed through Bernoulli numbers [2].*

1 Physical interpretation

We have: $t\equiv\varepsilon$ (energy of a single fermion of an ideal Fermi gas); $y\equiv\Theta=k_BT$ where k_B is the Boltzmann constant and T is the thermodynamic equilibrium temperature of the gas (therefore Θ is the temperature expressed in energy units); $f_1\left(y\right)\equiv\mu\left(\Theta\right)$ is the *chemical potential* of the gas. So the Fermi-Dirac integral can be rewritten:

$$F_D\left(\theta\right)=\int_0^{+\infty}\frac{\varphi\left(\varepsilon\right)d\varepsilon}{e^{\frac{\varepsilon-\mu(\theta)}{\theta}}+1}\tag{29}$$

The function $\varphi\left(\varepsilon\right)$ can be $g\left(\varepsilon\right)$ or $\varepsilon g\left(\varepsilon\right)$, where $g\left(\varepsilon\right)$ is the single fermion density of states[2]: $g\left(\varepsilon_0\right)d\varepsilon$ is the number of energy states $\varepsilon\in\left[\varepsilon_0,\varepsilon_0+d\varepsilon\right]$. If $\varphi\left(t\right)=g\left(\varepsilon\right)$, the Fermi-Dirac integral is the total number N of fermions in the gas. Since this number does not depend on the temperature Θ, we have the following normalization condition:

$$N=\int_0^{+\infty}\frac{g\left(\varepsilon\right)d\varepsilon}{e^{\frac{\varepsilon-\mu(\theta)}{\theta}}+1}\tag{30}$$

N doesn't depend on Θ

$$N=\left[\int_0^{+\infty}\frac{g\left(\varepsilon\right)d\varepsilon}{e^{\frac{\varepsilon-\mu(\theta)}{\theta}}+1}\right]_{\theta=0}=\int_0^{\varepsilon_F}g\left(\varepsilon\right)d\varepsilon$$

where $\varepsilon_F=\mu\left(0\right)$ it is the *Fermi energy* or the energy of the highest level occupied at the temperature of absolute zero. If $G\left(\varepsilon\right)$ è ithe number of energy states $\leq\varepsilon$ i.e. $g\left(\varepsilon\right)=\frac{dG(\varepsilon)}{d\varepsilon}$, then the functional relation $G\left(\varepsilon_F\right)=N$ uniquely defines the Fermi energy, and in cases where $G\left(\varepsilon_F\right)=N$ can be made explicit, it allows us to determine ε_F as a function of the

[2]This quantity is determined starting from the Hamiltonian of a single fermion. The simplest case is that of a gas not subjected to external force fields.

number N of fermions and therefore, of the density of the number of fermions. It turns out that ε_F increases as the fermion concentration increases. In this case, the limit $\Theta \ll \varepsilon_F$ which allows applying the Sommerfeld theorem (8) is also verified for Θ in the room temperature range[3]. This circumstance occurs for the conduction electrons of a metal which with good approximation make up an ideal Fermi gas. More precisely, the total energy of an ideal Fermi gas is obtained by assuming $\varphi(\varepsilon) = \varepsilon g(\varepsilon)$

$$E(\Theta) = \int_0^{+\infty} \frac{\varepsilon g(\varepsilon)\, d\varepsilon}{e^{\frac{\varepsilon - \mu(\theta)}{\theta}} + 1} \tag{31}$$

In the strong degeneracy limit ($\Theta \ll \varepsilon_F$) the Sommerfeld expansion for $E(\Theta)$ is:

$$E(\Theta) = \int_0^{\mu(\Theta)} \varepsilon g(\varepsilon)\, d\varepsilon + 2\Theta \sum_{k=1}^{+\infty} \Theta^{2k} \left[\frac{d^{2k-1}}{dx^{2k-1}} (\varepsilon g(\varepsilon)) \right]_{\varepsilon = \mu(\Theta)} \left(1 - 2^{1-2k}\right) \zeta(2k) \tag{32}$$

The first integral is the contribution to the total energy coming from fermions having energy $\leq \mu(\Theta)$. The series, however, expresses the contribution coming from fermions with energy $\geq \mu(\Theta)$. The kth term of the series is proportional to $\zeta(2k)$.

References

[1] Landau L.D. , Lifsits E.M., Fisica statistica. Editori Riuniti

[2] Edwards H.M., *Riemann's Zeta Function*. Dover Publications, inc. Mineola, New York.

[3] In general, for a temperature range $\Theta < \varepsilon_F$, the Fermi gas is said to be *degenerate* in the sense that it exhibits a deviation from the behavior predicted by classical statistical mechanics. If $\Theta \ll \varepsilon_F$, the gas is *strongly degenerate* and for $\Theta = 0$ it is *totally degenerate*.