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

\[
f : \mathbb{R}^+ \rightarrow \mathbb{R}^+ \quad t \mapsto f(t), \quad \forall t \in \mathbb{R}^+
\]

Precisely, \( f \) is the Fermi-Dirac function:

\[
f (t, y) = \frac{1}{e^{t/f_1(y)} + 1}
\]

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

\[
\Lambda (t) = \lim_{y \to 0^+} f (t, y)
\]

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

\[
\lim_{y \to 0^+} \frac{t - f_1 (y)}{y} = \begin{cases} 
-\infty, & 0 \leq t \leq t_0 \\
+\infty, & t > t_0
\end{cases}
\]

so

\[
\Lambda (t) \equiv f (y, 0) = \begin{cases} 
\frac{1}{e^{t/f_1(y)} + 1} = 1^-, & 0 \leq t \leq t_0 \\
\frac{1}{e^{t/f_1(y)} + 1} = 0^+, & t > t_0
\end{cases}
\]

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

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

\[ F_D(y) = \int_0^{+\infty} \varphi(t) f(t, y) \, dt \quad (6) \]

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):

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

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:

\[ F_D(y) = \Phi(f_1(y)) + 2y \sum_{k=1}^{+\infty} u_k(y) \quad (8) \]

where:

\[ \Phi(t) = \int_0^t \varphi(t') \, dt' \quad (9) \]

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

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

Dimostrazione. Performing the variable change:

\[ x = \frac{t - f_1(y)}{y} \quad (10) \]

The integral (7) becomes:

\[ F_D(y) = y \int_{-f_1(y)/y}^{+\infty} \frac{\varphi(f_1(y) + xy) \, dx}{e^x + 1} \quad (11) \]

For the decomposition property:

\[ F_D(y) = y \left[ \int_{-f_1(y)/y}^{0} \frac{\varphi(f_1(y) + xy) \, dx}{e^x + 1} + y \int_{0}^{+\infty} \frac{\varphi(f_1(y) + xy) \, dx}{e^x + 1} \right] \quad (12) \]

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

\[ I_1(y) = \int_0^{f_1(y)/y} \frac{\varphi(f_1(y) - x' y) \, dx'}{e^{-x'} + 1} \]
Redefining the mute variable $x'$

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

(13)

Furthermore

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

which when replaced (13) returns

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

(14)

where

$$I_2 (y) \overset{\text{def}}{=} \int_0^{f_1 (y) \over y} \varphi (f_1 (y) - xy) \, dx$$

(15)

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

$$I_2 (y) = \int_0^{f_1 (y) \over y} \varphi (f_1 (y) + xy) \, dx$$

(16)

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

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

(17)

Replacing (17) in (14):

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

(18)

From (12):

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

(19)

Replacing (18) in (19):

$$F_D (y) = \int_0^{f_1 (y) \over y} \varphi (t) \, dt - y \int_0^{f_1 (y) \over y} \varphi (f_1 (y) - xy) \, dx \, e^{-x + 1}$$

$$+ \int_0^{+\infty} \varphi (f_1 (y) + xy) \, dx \, e^{-x + 1}$$

(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:

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

(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:

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

Calculating the derivatives

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

e.g.

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

which replaced in (21):

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

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

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

We write

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

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

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

which replaced in (23):

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

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

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

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:
\[ \sum_{n=1}^{+\infty} \frac{(-1)^n}{n^\sigma} = (1 - 2^{1-\sigma}) \zeta(\sigma) \quad (26) \]
where \( \zeta(\sigma) \) is the Riemann zeta function \([2]\). In tal modo otteniamo la seguente espressione per \( J(\sigma) \)
\[ J(\sigma) = (1 - 2^{1-\sigma}) \Gamma(\sigma) \zeta(\sigma), \quad \forall \sigma > 0 \quad (27) \]
In particular
\[ \int_0^{+\infty} \frac{x^{2k-1}}{e^x + 1} \, dx = (1 - 2^{1-2k}) (2k - 1)! \zeta(2k) \quad (28) \]
because \( \Gamma(2k) = (2k - 1)! \). The statement follows from the substitution of (28) in (22).

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

## 1 Physical interpretation

We have: \( t \equiv \varepsilon \) (energy of a single fermion of an ideal Fermi gas); \( y \equiv \Theta = k_B T \) where \( k_B \) is the Boltzmann constant and \( T \) is the thermodynamic equilibrium temperature of the gas (therefore \( \Theta \) is the temperature expressed in energy units); \( f_1(y) \equiv \mu(\Theta) \) is the chemical potential of the gas. So the Fermi-Dirac integral can be rewritten:
\[ F_D(\theta) = \int_0^{+\infty} \frac{\varphi(\varepsilon) \, d\varepsilon}{e^{\frac{\varepsilon - \mu(\theta)}{\theta}} + 1} \quad (29) \]
The function \( \varphi(\varepsilon) \) can be \( g(\varepsilon) \) or \( \varepsilon g(\varepsilon) \), where \( g(\varepsilon) \) is the single fermion density of states\(^2\): \( g(\varepsilon_0) \, d\varepsilon \) is the number of energy states \( \varepsilon \in [\varepsilon_0, \varepsilon_0 + d\varepsilon] \). If \( \varphi(t) = g(\varepsilon) \), the Fermi-Dirac integral is the total number \( N \) of fermions in the gas. Since this number does not depend on the temperature \( \Theta \), we have the following normalization condition:
\[ N = \int_0^{+\infty} \frac{g(\varepsilon) \, d\varepsilon}{e^{\frac{\varepsilon - \mu(\theta)}{\theta}} + 1} \quad (30) \]
\( N \) doesn’t depend on \( \Theta \)
\[ N = \left[ \int_0^{+\infty} \frac{g(\varepsilon) \, d\varepsilon}{e^{\frac{\varepsilon - \mu(\theta)}{\theta}} + 1} \right]_{\theta=0} = \int_{\varepsilon_F}^{+\infty} g(\varepsilon) \, d\varepsilon \]
where \( \varepsilon_F = \mu(0) \) it is the Fermi energy or the energy of the highest level occupied at the temperature of absolute zero. If \( G(\varepsilon) \) è the number of energy states \( \leq \varepsilon \) i.e. \( g(\varepsilon) = \frac{dG(\varepsilon)}{d\varepsilon} \), then the functional relation \( G(\varepsilon_F) = N \) uniquely defines the Fermi energy, and in cases where \( G(\varepsilon_F) = N \) can be made explicit, it allows us to determine \( \varepsilon_F \) 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 $\varepsilon_F$ 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 $\Theta$ 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 $\varphi(\varepsilon) = \varepsilon g(\varepsilon)$

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

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

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

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 $k$th term of the series is proportional to $\zeta(2k)$.

References


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$^3$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.