An atypical case of round-off in *Mathematica*®

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Abstract

A Mathematica round-off case generated by a real function of a real variable, not elementary expressible.

1 Introduction

In semiconductor physics, the calculation of the *chemical potential* $\mu(T)$ [1], as a function of the thermodynamic equilibrium temperature T, is fundamental. This quantity solves a transcendent functional equation

$$F(T,\mu) = 0 \tag{1}$$

which can be made algebraic with the change of variable $z = k_B T \ln \mu$, where k_B is the Boltzmann constant, and the new quantity z is the *fugacity*. So

$$G(T,z) = 0 \tag{2}$$

Despite its algebraic character, (2) cannot be solved in closed form; solving numerically with *Mathematica* [2] we obtain the graph in Figure 1. Violent oscillations can be rarefied but not damped, using the `MaxRecursion` instruction as shown in Figure 1, while in Figure 3 we have reduced the thermal range to $[0,10]$. From this last graph we see that the *Mathematica* kernel is unable to graph $\mu(T)$ for $T<2$. However, it seems to be

$$\lim_{T\to 0} \mu(T) = 0$$

On the contrary, it is well known that the aforementioned limit is <0.

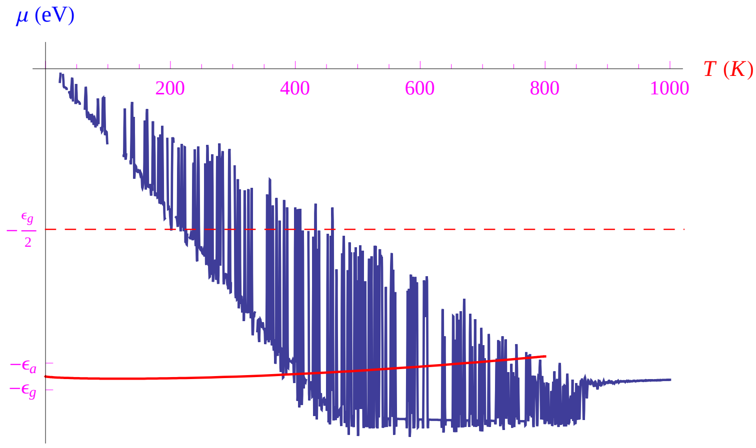

Figure 1: The curve in red is the solution obtained in a right neighborhood of $T=0$. The rapid swings are due to the *Mathematica* round-off.

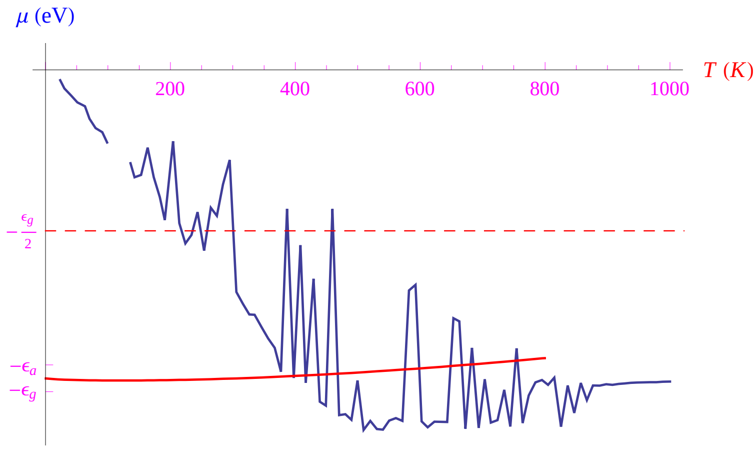

Figure 2: Reduction of oscillations by placing `MaxRecursion -> 1`.

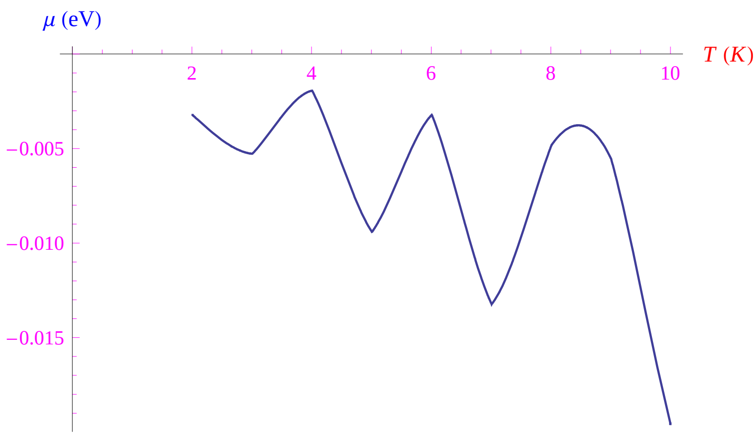

Figure 3: Trend for $T \in [0, 10]$.

2 Change of variable. Setting the problem

Definendo $x = k_B T$ ed espressa in eV, dopo aver posto $f(x) \equiv z\left(\frac{x}{k_B}\right)$ con $k_B = 8.62 \times 10^{-5}\,\text{eV}\,\text{K}^{-1}$, il nostro problema è:

Problem 1 *Let $f(x) > 0$ in $(0, +\infty)$ and such that*

$$\alpha_e x^{3/2} f(x) + \frac{\lambda f(x)}{f(x) + e^{-\frac{a}{x}}} = \alpha_h x^{3/2} \frac{e^{-\frac{b}{x}}}{f(x)} \tag{3}$$

where $b > a > 0$, while $\lambda \geq 0$ is a free parameter. $\alpha_e, \alpha_h > 0$ are expressed through Planck's reduced constant. Typical values: $\alpha_e = 1096.24$, $\alpha_h = 2013.92$.

Show:

1. *For $x \to 0^+$, $f(x)$ is an infinitesimal of infinitely large order. Furthermore, $f \in C^\infty(0, +\infty)$, $f \notin C^\omega(0, +\infty)$, meaning that $f(x)$ is continuous together with the derivatives of high order, but is not analytic.*

2. *$\lim_{x \to 0^+} x \ln f(x) = -\frac{a+b}{2}$.*

[Hint: for $0 < x \ll 1$ neglect $x^{3/2} f(x)$]

Soluzione

Question 1

For $\lambda = 0$ the (3) admits the only solution:

$$f(x) = \sqrt{\frac{\alpha_h}{\alpha_e}} e^{-\frac{b}{2x}} \tag{4}$$

which is manifestly an infinitesimal of infinitely large order for $x \to 0^+$:

$$\lim_{x \to 0^+} x^\alpha f(x) = 0, \quad \forall \alpha > 0$$

The same result is reached for the derivative $f^{(n)}(x)$. Extending these functions by continuity at the point $x = 0$, we have that $f \in C^\infty$, however it is not analytic at $x = 0$, since $f^{(n)}(0) = 0$, $\forall n$. It follows that the Taylor expansion of $f(x)$ with initial point x=0 returns the function identically zero, while in a right neighborhood of $x = 0$ it is $f(x) = 0$. Furthermore

$$g(x) \stackrel{def}{=} x \ln f(x) = -\frac{b}{2} + \frac{x}{2} \ln\left(\frac{\alpha_h}{\alpha_e}\right) \tag{5}$$

which, unlike f, is class-based C^ω.

For $\lambda > 0$ we observe that the (3) is a third degree equation in $f(x)$ that cannot be solved in closed form. For $0 < x \ll 1$ its solutions behave like that of the quadratic equation in $f(x)$:

$$\frac{\lambda f(x)}{f(x) + e^{-\frac{a}{x}}} = \alpha_h x^{3/2} \frac{e^{-\frac{b}{x}}}{f(x)} \tag{6}$$

Solving:

$$f_\pm(x) = \frac{\alpha_h}{2\lambda} x^{3/2} e^{-\frac{b}{x}} \left(1 \pm \sqrt{1 + \frac{4\lambda}{\alpha_h} \frac{e^{\frac{b-a}{x}}}{x^{3/2}}}\right) \tag{7}$$

The problem (1) requires $f(x)>0$, so

$$f\left(x\right)=\frac{\alpha_h}{2\lambda}x^{3/2}e^{-\frac{b}{x}}\left(1+\sqrt{1+\frac{4\lambda}{\alpha_h}\frac{e^{\frac{b-a}{x}}}{x^{3/2}}}\right) \tag{8}$$

For the calculation of $\lim_{x\to 0^+} f\left(x\right)$ we observe that

$$\lim_{x\to 0^+} x^{3/2}e^{-\frac{b}{x}}=0, \quad \lim_{x\to 0^+}\frac{e^{\frac{b-a}{x}}}{x^{3/2}} \underset{b>a}{=} +\infty$$

so that $\lim_{x\to 0^+} f\left(x\right)=0\cdot\infty$. This indetermination can be removed by observing that in a right neighborhood of $x=0$ of arbitrarily small radius it succeeds $\frac{e^{\frac{b-a}{x}}}{x^{3/2}}\gg 1$ since this ratio diverges positively for $x\to 0^+$. From this it follows that in the radicand of (8) we can neglect 1 with respect to the other term:

$$0<x\ll 1 \Longrightarrow f\left(x\right)\simeq\frac{\alpha_h}{2\lambda}x^{3/2}e^{-\frac{b}{x}}\left(1+\frac{2\lambda^{1/2}}{\alpha_h^{1/2}}\frac{e^{\frac{b-a}{2x}}}{x^{3/4}}\right)$$

In the same way $\frac{e^{\frac{b-a}{2x}}}{x^{3/4}}\gg 1$ in the same right neighborhood as $x=0$. In this order of approximation we have:

$$0<x\ll 1 \Longrightarrow f\left(x\right)\simeq\left(\frac{\alpha_h}{\lambda}\right)^{1/2}x^{3/4}e^{-\frac{a+b}{2x}} \tag{9}$$

So

$$\lim_{x\to 0^+} f\left(x\right)=\left(\frac{\alpha_h}{\lambda}\right)^{1/2}\lim_{x\to 0^+} x^{3/4}e^{-\frac{a+b}{2x}}=0^+ \tag{10}$$

Since in a right neighborhood of $x=0$ with a small radius, the function $f(x)$ is expressed as the product of an infinitesimal of order 3/4 by an infinitesimal of infinitely large order, we have that $f(x)$ is in turn an infinitesimal of infinitely large order. By calculating the derivatives of however high order, we arrive at the same result. We conclude that $f(x)$ is not analytic at $x=0$.

Question 2

From (9) it follows that in a right neighborhood of $x=0$ we have that $g(x)=xlnf(x)$ is expressed as

$$g\left(x\right)\simeq x\ln\left[\left(\frac{\alpha_h}{\lambda}\right)^{1/2}x^{3/4}e^{-\frac{a+b}{2x}}\right]=\frac{3}{4}-\frac{a+b}{2}+\frac{x}{2}\ln\left(\frac{\alpha_h}{\lambda}\right)$$

so

$$\lim_{x\to 0^+} g\left(x\right)=-\frac{a+b}{2} \tag{11}$$

To establish the possible presence of the round-off, we plot the graph of $g\left(x\right)$ in $[x_{\min}=k_B T_{\min}, x_{\max}=k_B T_{\mathrm{i}}$ where $T_{\min,\max}$ define the thermal range assigned in the section (1). It follows $x_{\min}=8.62\cdot 10^{-6}\,\mathrm{eV}$, $x_{\max}=0.086\,\mathrm{eV}$.

In Figure 4 Let's plot the graph of the function $g\left(x\right)=x\ln f\left(x\right)$ with $f\left(x\right)$ obtained by numerically solving the equation (3) and compared with the solution for $x\ll 1$ i.e. $g\left(x\right)=x\ln f\left(x\right)$ with $f\left(x\right)$ given by (8). We see, therefore, that the change of variable $T\to x=k_B T$ dampened the round-off oscillations. However, the latter is still present because according to the *Mathematica* kernel is $\lim_{x\to 0^+} g\left(x\right)=0$ contrary to the (11).

3 Conclusions

The round-off is triggered by the parameter $\lambda>0$, since for $\lambda=0$ the solution $f(x)$ is elementary expressible. Values $\lambda>0$ destroy the possibility of analytically solving the (3) and the corresponding solution is not elementary expressible.

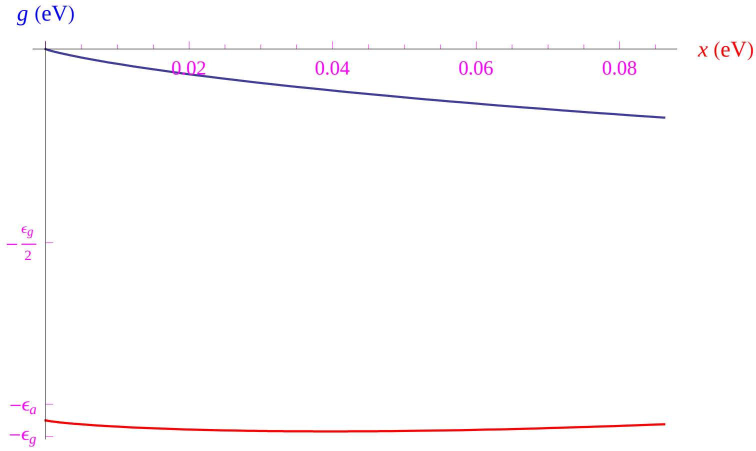

Figure 4: The curve in red is the graph of $g(x) = x \ln f(x)$ where the function $f(x)$ is given by (8). The curve in blue is the graph of g(x)=xln f(x) with $f(x)$ solution of the (3).

References

[1] Kittel C. Kroemer H. Termodinamica statistica.

[2] Wolfram S. *An Elementary Introduction to the Wolfram Language*.

[3] Wagon S. *Mathematica in Action*. Springer