21st INTERNATIONAL METROLOGY CONGRESS

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Theoretical and numerical studies of the Brillouin function and its inverse

Introduction

The Brillouin function, and its classical limit the Langevin function, and their inverses, are commonly employed in statistical and quantum mechanical studies of the magnetization of idealised paramagnetic and ferromagnetic materials. The Brillouin function is used to describe the dependence of the magnetic field on the total angular momentum J of the material.

The Brillouin function is defined by

$$\mathfrak{B}_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{1}{2J}x\right)$$

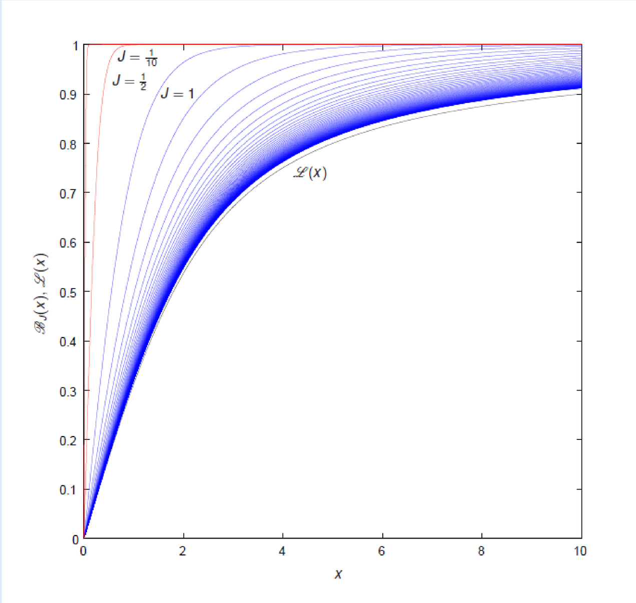
where J is the total angular momentum, which may take the values $0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$. This has the series expansion

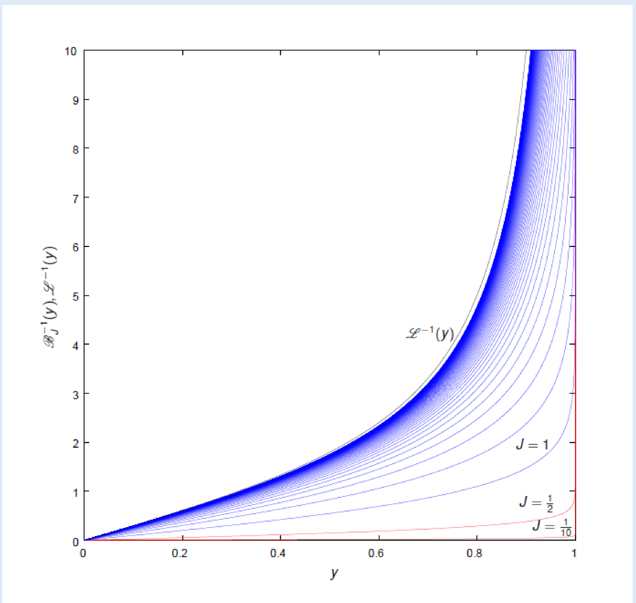
$$\mathfrak{B}_J(x) = \frac{J+1}{3J}x + \frac{J+1}{90J^3}(2J^2+2J+1)x^3 + \frac{J+1}{7560J^5}(4J^2+6J+3)(4J^2+2J+1)x^5 + O(x^7).$$

The Brillouin function can be re-expressed in terms of the Langevin function as

$$\mathfrak{B}_J(x) = \frac{2J+1}{2J}\mathfrak{L}\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\mathfrak{L}\left(\frac{1}{2J}x\right).$$

The inverse Langevin and Brillouin functions cannot be expressed in closed form and therefore many approximations have been developed to facilitate its application in many theoretical models.





In the classical limit $J \to \infty$, $\mathfrak{B}_J(x) \to \mathfrak{L}(x)$, the Langevin function which is defined by $\mathfrak{L}(x) = \coth x - 1/x$.

Analysis of the Brillouin function and its inverse

The poles of the Brillouin function

It proves convenient to rewrite the Brillouin function in the form

$$\mathfrak{B}_J(x) = \frac{N+1}{N}\coth\left(\frac{N+1}{N}x\right) - \frac{1}{N}\coth\left(\frac{1}{N}x\right), \qquad (1)$$

where $N = 2J = 1,2,3,\ldots$ ranges over all positive integers.

There is one possible pole for each pole of each $\coth$ term. The poles of $\coth x$ occur on the imaginary axis at the zeros of $\sinh x$, the two nearest to the origin being at $x = \pm\pi i$. The value $x = 0$ is a removable singularity as is clear from its series expansion. These possible poles occur at

$$\frac{N+1}{N}x = m'\pi i, \qquad \frac{1}{N}x = m\pi i,$$

where m' and m are integers.

The convergence is only up to the smallest radius of convergence, namely,

$|x| < \frac{N}{N+1}\pi$ i.e. $|x| < \frac{1}{2}\pi$ for $N = 1$, $|x| < \frac{2}{3}\pi$ for $N = 2$, etc..

We can demonstrate the following inequalities

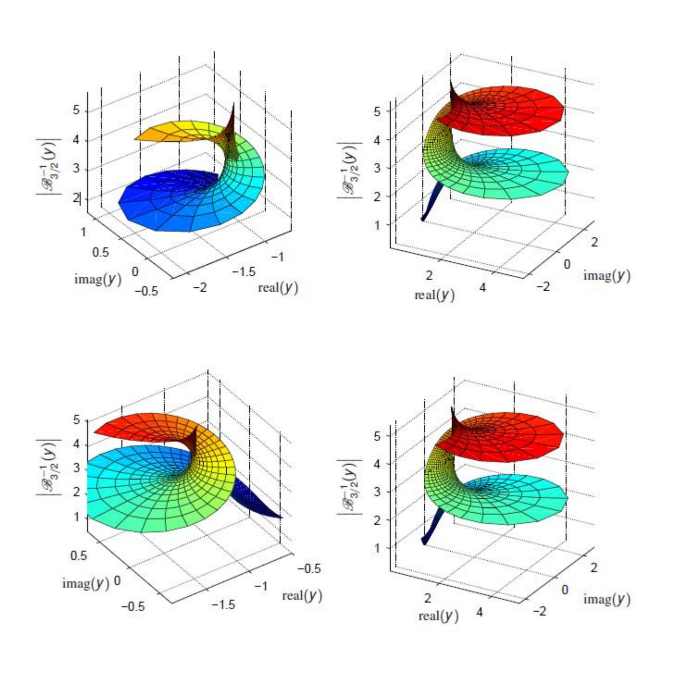
$$\mathfrak{L}(x) \equiv \mathfrak{B}_\infty(x) < \mathfrak{B}_{J_1}(x) < \mathfrak{B}_{J_2}(x) < 1 \equiv \mathfrak{B}_0(x)$$

for $0 < J_2 < J_1 < \infty$ and $x > 0$.

Exact results

For $J = 1/2$ the exact result is given by $\mathfrak{B}_{1/2}^{-1}(y) = \tanh^{-1}(y) = \frac{1}{2}\log\frac{1+y}{1-y}$.

For $J = 1$ the exact result is given by $\mathfrak{B}_1^{-1}(y) = \log\frac{y+\sqrt{4-3y^2}}{2(1-y)}$.



Plot of the four complex conjugate singularities for $\mathfrak{B}_{3/2}^{-1}(y)$ nearest the origin at $y = \pm 1.110063558 \pm 0.1000943686i$.

The inverse and reduced inverse Brillouin function

The inverse Brillouin function has series expansion

$$\mathfrak{B}_J^{-1}(y) = \frac{3J}{J+1}y + \frac{9J(2J^2+2J+1)}{10(J+1)^3}y^3 + \frac{27J(88J^4+176J^3+196J^2+108J+27)}{1400(J+1)^5}y^5 + O(y^7).$$

We may remove the logarithmic singularities as $y \to \pm 1$ from $\mathfrak{B}_J^{-1}(y)$ by defining a reduced inverse Brillouin function $F_J(y)$ by

$$F_J(y) = \mathfrak{B}_J^{-1}(y) - J\log\frac{1+y}{1-y}.$$

We see that $F_J(y)$ has series expansion

$$F_J(y) = -\frac{J(2J-1)}{J+1}y - \frac{J(2J-1)}{30(J+1)^3}(10J^2+8J+7)y^3 - \frac{J(2J-1)}{1400(J+1)^5}(280J^4+352J^3+600J^2+454J+169)y^5 + O(y^7).$$

Critical points for the inverse Brillouin function

Critical points occur when the derivatives either vanish or become infinite. We wish to investigate the critical points of $x = \mathfrak{B}_J^{-1}(y)$ which occur when $\frac{dx}{dy} = 0$ or ∞. Now

$$\frac{dx}{dy} = \frac{1}{dy/dx} \Rightarrow \frac{d}{dy}\mathfrak{B}_J^{-1}(y) = \frac{1}{d\mathfrak{B}_J(x)/dx},$$

we can find $d\mathfrak{B}_J(x)/dx$ by differentiating (1) to obtain

$$\frac{d\mathfrak{B}_J(x)}{dx} = -\frac{\left(\frac{N+1}{N}\right)^2}{\sinh^2\left(\frac{N+1}{N}x\right)} + \frac{\left(\frac{1}{N}\right)^2}{\sinh^2\left(\frac{1}{N}x\right)}.$$

The singularities occur for those values of x satisfying

$$\sinh\left(\frac{N+1}{N}x\right) + (N+1)\sinh\left(\frac{1}{N}x\right) = 0, \sinh\left(\frac{N+1}{N}x\right) - (N+1)\sinh\left(\frac{1}{N}x\right) = 0.$$

Program to calculate polynomial fit to the reduced inverse Brillouin function

- The program is based on the use of the Brillouin function $\mathfrak{B}_J$ with range $[-1,1]$ which we divide approximately into the regions $[-0.9999, -0.99]$, $[-0.99, 0.99]$ and $[0.99, 0.9999]$.
- We first consider the range $[-0.99, 0.99]$ of the Brillouin function and derive a minimal value of x that would allow us to define its corresponding domain $[-x_{\min}, x_{\min}]$.
- For each division in the calculated domain $[-x_{\min}, x_{\min}]$ we derive values corresponding to the range of the Brillouin function $[\mathfrak{B}_J(-x_{\min}), \mathfrak{B}_J(x_{\min})] \approx [-0.99, 0.99]$.
- Using the argument $\mathfrak{B}_J^{-1}(\mathfrak{B}_J(x)) = x$ we define the inverse Brillouin function with domain $[\mathfrak{B}_J(-x_{\min}), \mathfrak{B}_J(x_{\min})]$ and corresponding range $[-x_{\min}, x_{\min}]$.
- To remove the logarithimic singularities at $y \to \pm 1$ we employ the function
- $J\log((1+y)/(1-y))$ again with domain $[\mathfrak{B}_J(-x_{\min}), \mathfrak{B}_J(x_{\min})]$.
- Each region is fitted using a polynomial of the form $a_1x + a_3x^3 + a_5x^5 + \ldots$, the program continues to iterate increasing the size of the polynomial fit until the error of the region $[-0.99, 0.99]$ is within a specified accuracy. The degree of this polynomial is then used to curve fit the regions at the two extremes $[-0.9999, -0.99]$ and $[0.99, 0.9999]$.

J	[−0.9999, −0.99] Percentage Error	[−0.99, 0.99] Percentage Error	[0.99, 0.9999] Percentage Error	CPU Time (s)
1	0.001 %	0.0085 %	0.002 %	0.12
5	0.001 %	0.0069 %	0.001 %	0.12
10	0.001 %	0.0056 %	0.001 %	0.23
25	0.001 %	0.0099 %	0.001 %	0.44
50	0.001 %	0.0095 %	0.001 %	0.61
100	0.001 %	0.0052 %	0.001 %	2.04
250	0.001 %	0.0013 %	0.001 %	3.80
500	0.006 %	0.0025 %	0.007 %	4.38
1,000	0.044 %	0.0096 %	0.042 %	5.60
5,000	1.90 %	0.0089 %	1.90 %	7.07
10,000	4.15 %	0.0092 %	4.14 %	7.16
100,000	9.40 %	0.0096 %	9.36 %	7.21
1,000,000	9.97 %	0.0051 %	9.93 %	7.12

Calculated percentage errors for the polynomial fits when compared to the function $F_J(y)$

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