An application of the Cauchy problem in a semi-empirical context

Pardis Tabaee Damavandi

Queen Mary University of London, London, E1 4NS, UK

Copyright: © the author(s), publisher and licensee. This is an open-access article distributed under the terms of the Creative Commons Attribution Non-Commercial License, which permits unrestricted non-commercial use, distribution, and reproduction in any medium, provided the original work is properly cited.

Abstract: The Cauchy problem has been applied to a simple case of linear function in the form y=f(x) expressing wavelength values previously acquired through computer simulations and satisfying the observed empirical initial condition that the extrapolated value of the C-N torsion of 14.10 μm from the Spitzer Telescope spectrum should be sustained.

Introduction

The generic equation $y = 188.68\,x^{-1}$ (1) was previously found describing the "wavelength profile" of a rectangular hyperbola, which was obtained through a unit conversion of the vibrational dynamics calculations from the General Utility Lattice Program (GULP™) and compared with the experimental data available through the NASA database. [1]

Vibrational dynamics is of relevance because it increases accuracy and precision in the calculation of density of states that, when associated to empirical values, i.e. in the Spitzer Telescope measurements case demonstrate a clear fitting, proving that not only the telescope in question is as accurate too, but also that experiment and theory are highly similar.

It has been discussed for decades that computer simulations are therefore important in revealing information that can be predicted prior to experiments, and could eventually even replace experiments altogether.

Method

The Cauchy problem[2-3] has been applied on this occasion to explore solutions that satisfy the equation found $y = 188.68\,x^{-1}$ (1) as well as the condition imposed by the value of the Spitzer measurement (Table I), naturally, thus without the preoccupation that noise and other mathematical contaminants may play a role in the production of data.

$y= 188.68\ x^{-1}$ Wavelength Λ (μm)	Spitzer[3] Measurements λ (μm)	Standard deviation
94.33		
37.74		
18.87		
14.51	14.10	0.2926
(…)		

Table I. The table illustrates key modes obtained through the Gulp™ calculations, converted into wavelength and then compared to the Spitzer Telescope's measurement. The equation is found by plotting all the wavelengths.

$$\begin{cases} y' = 188.68\, x^{-1} \\ y(0.036) = 14.10 \end{cases} \tag{2}$$

Where the initial condition is set to the observed spectral value, and finally the integral is solved simply:

$$\begin{cases} y = \int 188.68\, x^{-1} dx \\ y(0.036) = 14.10 \end{cases} \tag{3}$$

in which *C* is the constant

$$\begin{cases} y = 188.68 \ln|x| + C \\ 14.10 = 188.68 \ln|0.036| + C \rightarrow \quad C = 641.32 \end{cases} \tag{4}$$

Therefore y(x) is the solution to the Cauchy Problem (Figure 1-2):

$$y(x) = 188.68 \ln|x| + 641.3 \tag{5}$$

which can be straightforwardly validated via derivation of the same.

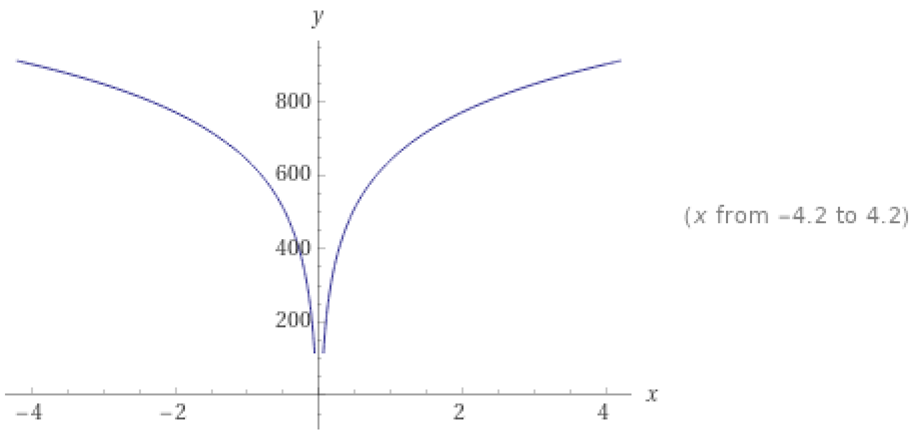

Figure 1. Plot for solution of equation $y' = 188.68\, x^{-1}$, where x falls within the interval of (-4.2 ; 4.2). Chart achieved by plotting via Wolfram Alpha [4].

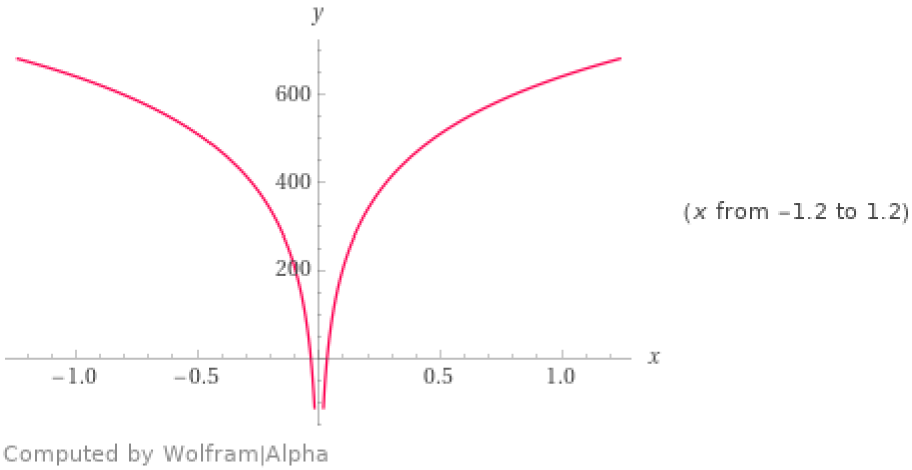

Figure 2. Plot for solution of equation $y' = 188.68\,x^{-1}$, where x falls within the interval of (-1.2 ; 1.2). Chart achieved by plotting via Wolfram Alpha [4].

Conclusion

The solution to the Cauchy Problem fulfils the set initial condition too, which defines the experimental value from the Spitzer Telescope measurement, satisfying the Peano existence theorem for ordinary differential equations as well.

Acknowledgments

Special thanks to Richard W. Pickersgill and Martin T. Dove.

References

1. Tabaee Damavandi, P., How to Detect Interstellar NT Glycine While Observing the Night Sky with an IR Telescope or IR Camera? *VIXRA preprint*, (2020). https://vixra.org/pdf/2005.0181v2.pdf
2. Bureau, F.J. Problems and methods in partial differential equations. *Annali di Matematica* 55, 323 (1961). https://doi.org/10.1007/BF02412091
3. Molteni, G., L-functions: Siegel-type theorems and structure theorems, February 1999. Ph.D. thesis. http://www.mat.unimi.it/users/molteni/research/tesi.pdf
4. Wolfram Alpha LLC. 2009. *Wolfram|Alpha*. http://www.wolframalpha.com/input/?i=2%2B2