Simulation of Heat Capacity at Low Temperatures

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May 9, 2025

Abstract

This report discusses a simulation of the low-temperature heat capacity of copper using a theoretical model that combines electronic and phononic contributions. By adding Gaussian noise to the simulated data and performing non-linear curve fitting, the key material parameters γ and β were extracted. The effectiveness of the model was evaluated using chi-square analysis, and limitations and future improvements are discussed.

1 Introduction

Heat capacity is a fundamental physical property that describes how much heat is required to change the temperature of an object. In introductory physics courses, students are introduced to the classic formula for heat, $q = mc\Delta T$, where c is the specific heat. This formula works well for everyday conditions as room temperature is high enough for quantum effects to be negligible. However, at extremely low temperatures, below ∼10 K, quantum effects become significant especially in metals.

At these low temperatures, quantum models are needed to accurately describe the heat capacity. The total heat capacity at constant volume, C_v, can be modeled as a sum of two distinct contributions. The first stems from lattice vibrations, phonons, which is described through the Debye model, with a predicted T^3 dependence. The second comes from the conduction electrons, which at low temperatures condense into a Fermi gas that contributes a linear temperature dependence.

$$C_v = C_{v,e} + C_{v,ph} = \gamma T + \beta T^3 \tag{1}$$

Here γ is the coefficient of the electronic contribution, and β represents the phonon contribution. Although the phonon term tends to dominate at higher temperatures, it becomes increasingly suppressed below 1 K and the electronic term becomes the dominant factor in heat capacity. A clever experiment technique involves dividing Eq. 1 by T and plotting C_v/T vs T^2 resulting in a linear graph:

$$\frac{C_v}{T} = \beta T^2 + \gamma \tag{2}$$

As we can see from Eq. 2 in this form γ now becomes the y-intercept and β gives the slope of the line [2]. This method allows for a straightforward extraction of the material-specific parameters. For this project, I simulate low-temperature heat capacity data for copper using this model. I wrote a code that produces data with noise, in an attempt to create realistic data, performed fits to extract the coefficients γ and β, and analyzed the fits to determine the quality of the simulation.

2 Methods

In order to simulate the low-temperature heat capacity of copper, I began with the theoretical expressions for heat capacity: Eq. 1 and Eq. 2. For the electronic contribution, I used a known experimental value for copper: $\gamma = 0.695$ mJ/mol·K^2 [2]. While β values were not as readily available, but it is possible to estimate β using the Debye model where the phonon contribution of heat capacity is related to the Debye temperature of the material. Since the Debye temperature for copper is well-established, $\theta_D = 343$ K, and using the low-temperature approximation of the Debye model (valid when $T \ll \theta$) to calculate β:

$$C_v \approx \frac{12\pi^4}{5} N k_B (\frac{T}{\theta})^3 \approx \beta T^3 \tag{3}$$

Here, Nk_B corresponds to the molar gas constant R, as we are working with molar quantities rather than individual particles. Substituting the known values into Eq. 3, I obtained an estimated value of $\beta = 4.82 \times 10^{-2}$ mJ/mol·K^4 [1].

In Python, I generated 50 evenly spaced temperature values ranging between 0.5-10 K. In an attempt to generate experimental-like data, I included small random fluctuations in temperature to simulate instrument sensitivity and uncertainty in measurements at low temperatures. Using the theoretical equations, heat capacity values were computed and Gaussian noise was added to these values to simulate measurement error. This process was repeated within a loop to simulate multiple trials of the experiment, and calculated the mean and standard deviation values of C_v and C_v/T at each temperature, before saving these into corresponding arrays. This data was then tabulated for easy visualization and comparison.

To extract the physical parameters γ and β, I performed least-square curve fits on both sets of data. Uncertainties on these values were determined using the covariance matrix of the fitting function. The mean data was then plotted vs their respective models, along with the printed parameter values.

A check of the simulations was performed by calculating the Debye temperature back from the fitted β values to ensure they still matched the inputted values from the start. Finally the chi-squared and reduced chi-squared values were calculated for both models to assess the goodness of fits.

3 Results

Due to the randomized noise introduced in each simulation, every trial yields slightly different data and fit outcomes.

Table 1: Fitted parameters and chi-squared values for C_v and C_v/T across five simulation trials.

C_v **Fit Results**					
Trial	β	γ	Debye	χ^2	Reduced χ^2
Original Values	0.696	.0482	343		
1	0.682	0.0487	341.68	141.52	2.95
2	0.687	0.0485	342.24	207.80	4.33
3	0.670	0.0488	341.53	298.60	6.22
4	0.702	0.0482	342.97	195.36	4.07
5	0.655	0.0490	340.94	434.71	9.06
Avg. Uncertainty	± 0.024	± 0.00032	± 0.754	–	–
C_v/T **Fit Results**					
Trial	β	γ	Debye	χ^2	Reduced χ^2
Original Values	0.696	.0482	343		
1	0.690	0.0485	342.25	18.83	0.39
2	0.693	0.0483	342.61	18.85	0.39
3	0.689	0.0484	342.39	34.77	0.72
4	0.696	0.0482	342.84	23.56	0.49
5	0.691	0.0484	342.52	22.92	0.48
Avg. Uncertainty	± 0.006	± 0.00012	± 0.31	–	–

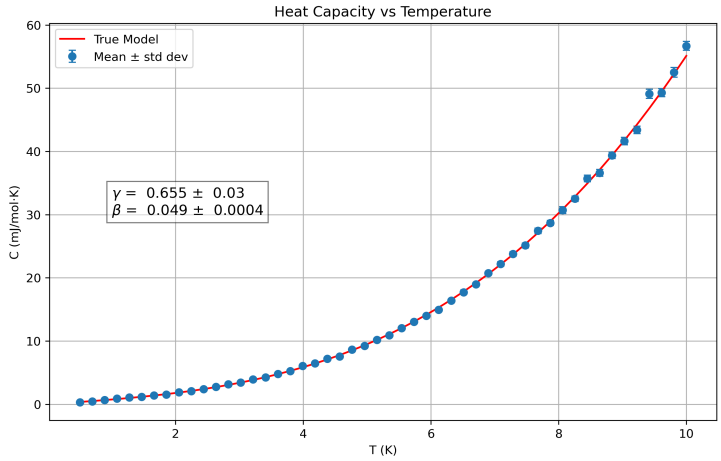

Figure 1: Plot of C_v vs T (trial 5)

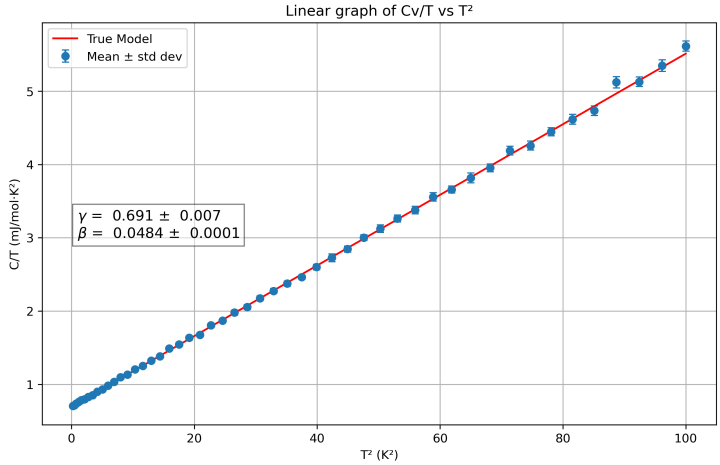

Figure 2: Plot of C_v/T vs T^2 (trial 5)

While the fitted parameters in Table 1 and the plots in figures 1 and 2 closely match the input values, the chi-squared values reveal important insight into the model's performance as well as the nature of the noise.

In the case of C_v, the lowest χ^2 value of the five trials was 141.52, which exceeds the 95% critical value of ~67.5 for 48 degrees of freedom. This suggests that the simulation does not fully account for the noise effects under the current model. The reduced χ^2 value further supports this as the lowest value 2.95, above the targeted value of 1, indicates poor agreement between the model and data.

In contrast, the C_v/T fits yields significantly lower χ^2 values, with the highest being 38.77, well below the critical value. However, the reduced χ^2 values were all below 1. While this could imply excellent fits, it more likely suggest overfitting of the data.

4 Conclusion

This project simulated low-temperature heat capacity data for copper using a Gaussian noise model to emulate experimental conditions and data. Although the model displayed limitations in its current state, the consistent ability to extract the original parameters of γ and β, as well as to recalculate the Debye temperature, validates the methodologies of this simulation. The conclusion is that the noise model was likely too simplistic for these extreme temperatures, especially considering the exponential temperature dependence in equations 1 and 2. Future work could include a more realistic noise model that scales with temperature, temperature-dependent error bars, and simulations with other metals for a comparative analysis.

References

[1] Ralph Baierlein. *Thermal Physics*. Cambridge University Press, 1999.

[2] Charles Kittel and Paul McEuen. *Introduction to Solid State Physics*. Wiley, 6th ed. edition, 2018.