Empirical formula for specific heat of solids based on atomic constants and a universal subzero limiting temperature

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Abstract. We present a novel empirical approach to understand the specific heat capacities of solids by introducing a characteristic subzero reference temperature derived from fundamental atomic constants. Using the total energy of the electron associated with the Bohr radius and the proton-electron mass ratio, we define a universal lower temperature limit as 3.87862×10^{-14} K. Based on this temperature and a room temperature of 300 K, we propose a simple empirical relation for specific heat capacity expressed in terms of atomic mass number A: $C = 25416.852/A$ J/kg.K. The formula accurately predicts experimental specific heat capacities across various elemental solids, providing a fundamental link between atomic-scale constants and macroscopic thermodynamic behaviour. Considering 'grams to kilograms' and 'moles to kilomoles' and with reference to Dulong-Petit law, it can be expressed as, $C = [3 \times 1000 \times R]/A$. It needs further study.

1 Introduction

Thermal energy point of view, one of the most important, inherent and intrinsic property of any material is its 'Specific Heat Capacity'(SHC). It is generally defined as the thermal energy absorbed by any material per unit mass per degree increase in temperature. It is well established that, atomic rotational and vibrational modes carry heat and raise the temperature of any substance. In all scientific and engineering applications, SHC is having a very crucial role. In this context, we would like to emphasize the point that, current physical models are lagging in understanding the basics of SHC in view of atomic physical constants. Mostly they are semi-empirical and phenomenological models having different advantages and limitations [1]. For example,

1) According to the Dulong-Petit law [2], SHC of atomic solids is approximately constant at $3R$ (where R is the gas constant). Considering atoms as classical harmonic oscillators, Boltzmann explained this law.
2) Einstein's quantum model assumes 'atoms' as quantum harmonic oscillators [3].

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3) Considering atomic vibrations as phonons, Debye successfully explained the SHC of solids at low temperatures [4].
4) Density functional theory [5] and modern machine learning methods are the advanced models having significant solutions [6,7].

2 Two assumptions and their possible applications

We would like to emphasize the point that there is a grey area in between 'thermal physics' and 'atomic physics'. In this contribution, to understand the origin of SHC of solids, in a unified approach, we introduce the following two new assumptions based on SI units.

1) Similar to the existence of 'quantum' of electric charge and magnetic flux, there exists a lower limit to the temperature near to sub-zero temperature.
2) Atomic mass number expressed in '*A* kg' plays a significant role in thermal physics.

2.1 About the first assumption

Considering the Bohr's atomic model and giving importance to the total energy of electron associated with the Bohr radius, we assume that,

$$T_{lower} \cong \frac{E_{Bohr}}{k_B\left[\exp\sqrt{m_p/m_e}\right]} \cong \frac{13.6\ \text{eV}}{k_B\left[\exp\sqrt{m_p/m_e}\right]} \cong 3.87862\times10^{-14}\ \text{K} \qquad (1)$$

where,
$T_{lower} \cong$ Defined lower limit of temperarure $\cong 3.87862\times10^{-14}$ K
$m_p \cong$ Rest mass of proton
$m_e \cong$ Rest mass of electron
$E_{Bohr} \cong$ Total energy of electron in the Bohr radius of Hydrogen atom
$k_B \cong$ Boltzmann's radiation constant

It may be noted that, 38 pico K is the current experimentally measured lower value [8] and is 980 times higher than our assumption. Considering this low temperature limit, it seems possible to define the quantum of thermal energy associated with low temperature physics, zero-point energy of quantum systems, minimum energy of photons associated with Wien's law, ending state of stellar objects, upper mass limit of black holes and ending state of the expanding universe. Interested readers and scholars can work on alternative lower temperature limits. Whatever may be the value of the lower temperature limit, qualitatively and quantitatively, it certainly helps in exploring the mystery of atoms' thermal behaviour.

2.2 About the second assumption

This concept seems to be in line with the currently believed notion of concept of '*A* gram' or 'gram mole' [9]. This assumption helps in connecting atoms and their massive thermal behaviour for "6.023×10^{26}" number of atoms. It is well established that, atomic mass number represented by the letter *A* plays an elemental role in generating the mass of any atom. It is also well established that, atomic mass plays a vital role in atoms' thermal behaviour. As discussed above, all the modern SHC models are lagging in connecting the

atomic physical constants and thermal physical constants. To bridge the gap, it seems necessary to implement the mass number in thermal physics.

3 An empirical relation for specific heat capacity of elementary solids

Based on the above two assumptions and considering the experimental values of SHC of atomic solids, we have developed an empirical relation. It is very simple to understand and easy to implement.

3.1 Proposed empirical formula

Considering 'room temperature' and the proposed lower temperature limit, we define a variable x in the following way.

$$x \cong \ln\left(\frac{T_{room}}{T_{lower}}\right) \cong \ln\left(\frac{300}{3.87862\times10^{-14}}\right) \cong 36.5845 \tag{2}$$

where T_{room} is the room temperature expressed in kelvin. Based on this logarithmic ratio, we try to fit the SHC of solids as,

$$C_A \cong \sqrt{1+x+\sqrt{x}}\left(\frac{M_u c^2}{T_{lower} A}\right) \cong \frac{25416.852}{A} \quad \frac{\text{J}}{\text{kg.K}} \tag{3}$$

It means,

$$C_A \propto \frac{M_u c^2}{T_{lower} A} \quad \text{and}$$

$$C_A \propto \sqrt{1+x+\sqrt{x}}$$

Where
- $C_A \cong$ Specific heat capacity of atomic solid in J/(kg·K)
- $M_u \cong$ Unified atomic mass unit in 'kg'
- $M_u c^2 \cong$ Rest energy of unified atomic mass unit in 'J'
- $T_{lower} \cong$ Defined lower limit of temperature in 'K'
- $A \cong$ Atomic mass number of the solid expressed in 'kg'

Note-1 : Based on our assumption 2, this relation is dimensionally consistent.

Note-2: Even though the factor $\sqrt{1+x+\sqrt{x}}$, is an ad hoc expression, it helps in fitting the SHC of atomic solids with marginal error. Interested scholars can modify this for a better understanding and accuracy.

3.2 Physics behind the empirical law

From the above formula, it is interesting to note that,

1) Atomic SHC is strongly coupled with the unified atomic unit.
2) SHC of atoms is inversely proportional to the mass of '*A* kg'.
3) Following '*A* kg mole' concept, 6.023×10^{26} number of atoms seem to have a common role in deciding the SHC of any atomic solid.
4) Tendency of atomic vibrations decrease with increasing mass of the atomic solid.
5) Sub-zero temperature limit is having a hidden and inherent role in deciding the SHC of atoms.

Based on these points, modern SHC models can be reviewed and revised for a better understanding at atomic level.

4 Experimental data and validation of the empirical formula

4.1 Different elements and their experimental and estimated values

Considering different metals having different crystal structures, different bonding characteristics, and different atomic masses, our proposed empirical formula can be validated with reference to their experimental SHC values [10]. One may consider the following different metals.

1) Light metals: Aluminium (Al)
2) Transition metals: Iron (Fe), Copper (Cu), Tungsten (W)
3) Noble metals: Silver (Ag), Gold (Au)
4) Heavy metals: Lead (Pb)

See the following Table 1 and Figure 1 for the estimated and experimental SHC of various solids.

Table 1. Comparison of predicted and experimental values of Specific heat capacity of solids.

Element	Atomic Mass Number A_rel	Predicted C (J/kg·K)	Experimental C (J/kg·K)	Difference (J/kg·K)	% Error
Aluminium (Al)	26.98	942	897	45	-5.0
Iron (Fe)	55.85	455	449	6	-1.3
Copper (Cu)	63.55	400	385	15	-3.9
Silver (Ag)	107.87	236	235	1	-0.4
Tungsten (W)	183.84	138	134	4	-3.0
Gold (Au)	196.97	129	129	0	0.0
Lead (Pb)	207.2	123	128	-5	3.9

4.2 Statistical analysis

One can find good agreement between the estimated and experimental values of SHC:

1) Mean absolute error: 11 J/(kg·K)
2) Mean relative error: 2.4%
3) Maximum error: 5.0% (Aluminium)

4) Perfect agreement: Gold (0% error)

These small percentage differences validate the proposed empirical formula's predictive power across a wide range of elements having different internal structures.

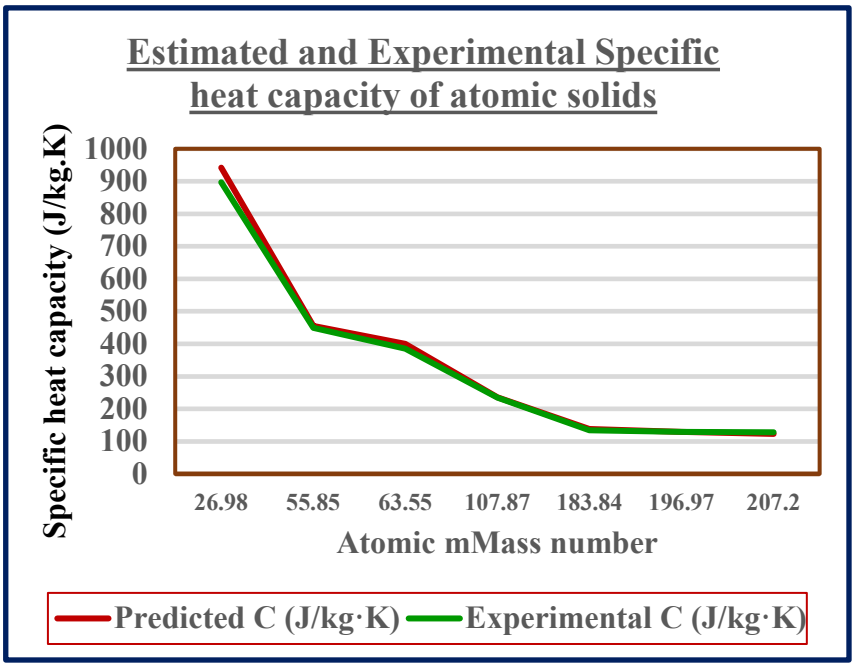

Fig. 1. Estimated and experimental values of Specific heat capacity of solids.

5 Discussion

5.1 Connection to stellar physics

Based on their mass, composition and evolution scheme, different star surface temperature ranges (STR) can be expressed as,

1) For M- type stars, STR is 2400 to 3700 K.
2) For K- type stars, STR is 3700 to 5200 K.
3) For G- type stars, STR is 5200 to 6000 K.
4) For F- type stars, STR is 6000 to 7600 K.
5) For A- type stars, STR is 7600 to 10000 K.
6) For B- type stars, STR is 10000 to 30000 K.
7) For O- type stars, STR is around 40000 K.

According to modern astrophysical observations, some stars have extraordinarily high surface temperatures in the range of (0.16 to 0.2) million-degree kelvin [11]. In this context, we have noticed that,

$$\left(T_{star}\right)_{high} \cong \left[\exp\left(\sqrt{\frac{m_p}{m_e}}\right)\right] T_{lower} \cong 0.16 \text{ Million K} \tag{4}$$

This observation can be considered as a supporting tool in validating our proposed low temperature limit. With further astrophysical studies and observations, proposed lower temperature limit can be reviewed and refined.

5.2 Bridging quantum mechanics and thermodynamics

According to quantum mechanics and quantum rules, there exists 'zero-point energy'. It seems to be a qualitative statement. Considering our low temperature limit, one can define the zero-point like 'quantum of thermal energy' as $\frac{1}{2}k_B T_{lower} \cong 2.68\times10^{-37}$ J. It can be considered as a reference of quantum-thermal energy constant at sub-zero thermal scale. Its ratio associated with actual thermal energy of physical systems and stellar objects can help in exploring the secrets of origin of thermal energy in a quantum thermodynamical approach.

5.3 Applications of the characteristic subzero temperature 3.88 × 10^{-14} K in physics

Considering this low temperature limit, various branches of physics and various engineering domains can be explored with respect to their minimum reachable temperature limits and various operating physical conditions. Various application domains are:

1) Quantum computing and information processing
2) Cryogenic engineering and superconductivity
3) Materials science and nanotechnology
4) Space technology and satellite applications
5) Cosmology and Astrophysics
6) Fundamental physics research

For example,

1) Quantum computing point of view, noise free operating temperature of low temperature range can be explored [12].
2) Thermal behaviour of super conducting materials and cryogenic systems can be explored.
3) Thermal properties of advanced semiconductors [13], thermoelectric devices and various quantum sensors can be studied for enhancing their operating environment.
4) Space technology point of view, ultra-low temperature sensors calibrated against the quantum reference temperature. It may help in thermal stability of deep-space missions in all aspects.
5) Cosmology point of view, fluctuations in cosmic microwave background radiation can be understood, ending stage of cosmic evolution [14] can be understood and dark matter origin can be understood.
6) Astrophysics point of view, compact astrophysical objects' birth secrets can be understood.

7) Following Hawking's blackhole temperature formula [15], upper limit a black hole can be estimated to be 3.2×10^{36} kg which can be expressed as 1.6 million solar masses.

5.4 Comparison with classical models

Compared to Dulong-Petit law, Einstein's quantum model and Debye's low temperature model, our assumptions and empirical formula, both, seem to have wide scope and in-depth physics. Application point of view, our approach is having, universality, simplicity, accuracy, physical foundation and computational ease.

5.5 Limitations and future directions

Even though our approach is having wide scope and accuracy, it is not directly applicable for liquids, gasses and other compound materials. Considering anharmonic effects and phase transitions, our approach needs a critical review. Its applicability and validity for 'above and below' the room temperature seems to be a failure. In this context, we have developed an 'approximate model' relation for a working temperature range of 100 to 800 K. With two adjustable coefficients *y* and *z,* it can be expressed as,

$$C_A \cong y\times\sqrt{1+x+\sqrt{x}}\left(\frac{M_u c^2}{T_{lower}A}\right)\ \frac{\text{J}}{\text{kg.K}} \tag{5}$$

$$\text{where}\begin{cases} y \approx z*\left(\dfrac{T_{\text{work}}}{T_{room}}\right)^{0.25} \\ z \cong A \text{ coefficient} \cong \ 0.85 \text{ to } 0.9 \\ T_{\text{work}} \cong \text{Working temperature} \\ T_{\text{room}} \cong \text{Room temperature} \end{cases}$$

Considering density functional theory and machine leaning methods along with the experimental data, it seems possible to modify this relation.

6 Comparison with Dulong-Petit law

The classical Dulong-Petit law [2] states that the molar heat capacity of solid elements is approximately constant at *3R*, where *R* is the universal gas constant. Numerically, this corresponds to about 24.94 J/mol·K in the molar quantity basis, generally expressed in CGS units. Our proposed empirical formula for specific heat capacity is given by, $\frac{25416.852}{A}\ \frac{\text{J}}{\text{kg.K}}$. To relate our constant with the classical Dulong-Petit constant, one must recognize the essential unit conversion factor resulting from the use of different definitions of the molar amount and mass:

a) In the CGS system, the mole corresponds to the quantity associated with 6.023×10^{23} particles and uses grams as the unit of mass.

b) In the SI system adopted in our approach [9], the kilomole (kmol) associated with 6.023×10^{26} particles is used, and kilograms is the unit of mass.

This difference means that the Avogadro number value in SI units is larger by a factor of 1000 compared to CGS units, and the mass unit is scaled correspondingly by 1000 (since 1 kg = 1000 g). Consequently, when converting the molar heat capacity from CGS (per mol) to SI (per kmol and per kg), a multiplication factor of 1000 appears. It may be noted that,

1. **Molar Heat Capacity**: Defined as the heat required to raise one mole of a substance by 1 K, with units typically given as J/mol·K.
2. **Specific Heat Capacity**: Defined as the heat required to raise one kilogram of a substance by 1 K, with units J/kg·K.
3. To convert molar heat capacity C_m to specific heat capacity C, use the molar mass M of the substance:

Let, $M \cong A \ \frac{gram}{mole}$

$$\begin{aligned} C_A &\cong \frac{C_m}{M} \cong \frac{C_m}{A} \ \frac{J}{\frac{gram}{mole}\times mole\times K} \\ &\cong \frac{C_m}{A} \ \frac{J}{\frac{gram}{mole}\times mole\times K}\left(\frac{1000}{1000}\right) \\ &\cong \frac{1000C_m}{A} \ \frac{J}{1000gram\times K} \cong \frac{1000\times 3R}{A} \ \frac{J}{kg\times K} \end{aligned} \tag{6}$$

7 Conclusion

Our proposed two assumptions, 'low temperature limit' and 'A kg mass' and the proposed empirical formula for specific heat capacity seem to work well for different elementary solids and paving a novel approach for bridging quantum mechanics and thermal physics at atomic level. Proceeding further, our proposed sub-zero temperature limit seems to have wide applications across all the branches of physics. Further studies will certainly help in exploring the missing physics applicable to specific heat capacity of solids, liquids, gasses and compound materials above and below the room temperature.

Data availability statement : The data that support the findings of this study are openly available.

Conflict of interest: Authors declare no conflict of interest in this paper or subject

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References

1. Souza, M.d., Paupitz, R., Seridonio, A. *et al.* "Specific Heat Anomalies in Solids Described by a Multilevel Model". *Braz J Phys* **46**, 206–212 (2016)
2. Roberto Piazza. "The strange case of Dr. Petit and Mr. Dulong". arXiv:1807.02270v1 [physics.hist-ph] (2018)
3. Coleman, P., Schofield, A.J., "Quantum criticality," Nature 433, 226–236 (2005).
4. Gonzalez, I.; Kondrashuk, I.; Moll, V.H.; Vega, A. Analytic Expressions for Debye Functions and the Heat Capacity of a Solid. Mathematics, 10, 1745 (2022)
5. Giustino, F., "Materials Modelling using Density Functional Theory," Nat. Rev. Phys. 3, 162–176 (2021).
6. Gusev, Y.V. "Experimental verification of the field theory of specific heat with the scaling in crystalline matter". Sci Rep **11**, 18155 (2021)
7. Maradudin, A.A., "Theory of Lattice Dynamics in the Harmonic Approximation," Academic Press (1963).
8. Yang, L, Villalobos, U, Akhmetov, B, Gil, A, Khor, JO, Palacios, A, Li, Y, Ding, Y, Cabeza, LF, Tan, WL & Romagnoli, A, "A comprehensive review on sub-zero temperature cold thermal energy storage materials, technologies, and applications: state of the art and recent developments", Applied Energy, 288, 116555 (2021)
9. Seshavatharam U. V. S, Gunavardhana Naidu T and Lakshminarayana S. "Avogadro's Number: History, Scientific Role, State-of-the-Art, and Frontier Computational Perspectives". Preprints **2025**, 2025080338.
10. Solids - Specific Heats. https://www.engineeringtoolbox.com/specific-heat-solids-d_154.html
11. Sander, A. A. C.; Hamann, W.-R.; Todt, H.; Hainich, R.; Shenar, T.; Ramachandran, V.; Oskinova, L. M.. "The Galactic WC and WO stars. The impact of revised distances from Gaia DR2 and their role as massive black hole progenitors". Astronomy and Astrophysics. 621: A92 (2019)
12. Blundell, S., "Magnetism in Condensed Matter," Oxford University Press (2001).
13. Rodríguez, I., Hinojosa-Romero, D., Valladares, A. et al. A facile approach to calculating superconducting transition temperatures in the bismuth solid phases. Sci Rep 9, 5256 (2019)
14. Adams, F.C., Laughlin, G., "A Dying Universe: The Long-Term Evolution of Astrophysical Objects," Rev. Mod. Phys. 69, 337–372 (1997).
15. Hawking, S.W., "Particle Creation by Black Holes," Commun. Math. Phys. 43, 199–220 (1975).