Thermal Properties of Diffusing Species into Some Host Metals

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Abstract: The study rigorously explored the thermodynamic properties of diffusing species by solving the spherical coordinate equation using the Frobenius method. This mathematical approach enabled the derivation of the partition function and energy equation, which were crucial in determining key thermal properties, including Helmholtz free energy, entropy, internal energy, and heat capacity. It was observed that internal energy and entropy exhibited a strong dependence on temperature, reflecting the dynamic nature of diffusing species in varying thermal environments. The findings provide valuable insights into the behavior of entropy within the classical domain, with both analytical expressions and graphical representations used to illustrate these thermal properties comprehensively. The graphical analysis highlighted the temperature-dependent trends and the critical points where classical and quantum mechanical effects influence the thermodynamic behavior of the system, offering a deeper understanding of the underlying physics.

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1.0   Introduction

The study of thermodynamic properties of diffusing species is highly relevant in both the physical and chemical sciences as it primarily deals with the relationship between temperature and energy. Thermodynamics plays a crucial role in high-energy physics, where at sufficiently high temperatures or densities, statistical quantum chromodynamics and nuclear matter may undergo a color-deconfined partonic phase (Abu-Shady *et al.,* 2016a). Thermodynamic properties are essential for describing quark-gluon plasma and for calculating heavy quarks in the context of strange quark matter (Inyang *et al.*, 2021a; Obu *et al.*, 2020). The increasing interest in the study of thermodynamic properties among researchers is a testament to its importance in various areas of physical and chemical sciences. The primary objective of studying these properties is to determine the partition function (PF), which serves as a foundation for deriving other thermodynamic properties (Inyang *et al.,* 2022; William *et al.,*2022). Notably, many researchers have explored the thermodynamic properties of different systems under various potentials. For example, Onate *et al*. (2021) and Okorire *et al.* (2021) have made significant contributions in this area. Abu-

Shady *et al*. (2016b) calculated the thermodynamic properties of heavy mesons, while Edet *et al*. (2021) investigated the thermal properties and magnetic susceptibility of the Hellmann potential in Aharonov-Bohm flux and magnetic fields at both zero and finite temperatures.

Over the last two decades, considerable efforts have been made to understand the structure and thermodynamics of several simple liquid metals, liquid transition metals, liquid rare-earth metals, and their alloys. While the interatomic potential of simple metals has been extensively studied, allowing for accurate derivation of their thermodynamic properties, the hybridization of d electron with s electron in transition metals introduces complexity (Nitin *et al.,* 2002). It is important to note that statistical thermodynamics, specifically the partition function, is crucial for determining the thermodynamic properties of any physical system (Inyang *et al.,* 2021b). The

thermodynamic properties can be broadly categorized into thermal functions and equations of state. Thermal functions relate the temperature of a substance to its internal energy and include properties such as enthalpy, entropy, and heat capacity. Equations of state, on the other hand, connect the density of a substance with its composition, pressure, and temperature, with key properties including isothermal compressibility and isobaric expansivity. The reactivity of a material depends on its chemical potential, which involves both thermal functions and equations of state (Charles & Lesher, 2015). This study, therefore, aims to analyze the thermodynamic properties of diffusing species using the Frobenius method.

2.0   Formalism

The procedures and steps that lead to this general equation of diffusing species into some host metals in spherical solids can be found in Ngangia *et al.* (2024).

$$C(c,t) = \frac{108D^2 n + 120Dn^2}{1620D^3 - 1935Dn + 204Dn^2 - 60n^3}\left[\left(1 - \frac{n}{6D}r^2\right) + \left(\frac{1}{r} - \frac{n}{2D}r\right)\right] + $$

$$\frac{90D^2 + 12Dn}{180D^2 - 15Dn + 6n^2}\left[r + \left(1 - \frac{n}{6D}r^2\right)\right] \tag{1}$$

where D is diffusion coefficient, n is a constant of value 0.5, r is the radius of the sphere measured in meter (m) and C is concentration measured in mole per meter cube ($mol..m^{-3}$).

2.1 Complimentary equations

The diffusion coefficient D (concentration-dependent system) is given by

$$D = D_0 e^{\beta_1 C} \tag{2}$$

where D is the diffusion coefficient for the surface concentration of the solids and β_1 is a constant. The diffusion coefficient (D) in

temperature-dependent systems which obeys the Arrhenius-type equation

$$D = D_o e^{\frac{-E_r}{KT}} \tag{3}$$

where E_r, T and D_O are the activation energy, temperature and
pre-exponential factor respectively.

2.2   Fractional Stokes-Einstein Model

According to Price *et al.* (2016), the Fractional Stokes-Einstein relation for the diffusion coefficient is given by

$$D = \frac{K_\beta T}{6\pi\mu r^\varepsilon} \tag{4}$$

where, $K_B = $ Boltzmann constant, μ is viscosity and r the radius of the sphere $\varepsilon < 1$ and ranges from 0.6 - 0.9.

3.0   Partition Function

Partition functions are functions of the thermodynamic state variables, such as temperature and volume (Akira *et al.,* 2015). Most of the aggregate thermodynamic variables of the system, such as total energy, free energy, entropy, and pressure, can be expressed in terms of the partition function or its derivatives. The partition function describes the statistical properties of a system in thermodynamic equilibrium. Each partition function is constructed to represent particular statistical ensembles (which, in turn, correspond to a particular free energy). Hence, any physical system with thermodynamic properties needs the introduction of the concept of partition function given by the expression (Okorie *et al.,* 2018).

$$Z_r(T) = \sum_{r=0,1}^{\infty} EXP - \left(\frac{E_r}{K_B T} \right) \qquad (5)$$

where, K_B = Boltzmann constant and T is temperature.

Equating equations (3) and (4) together gives

$$E_r = -RT \ln\left(\frac{K_B T}{D_0 6\pi\mu r^\varepsilon} \right) \qquad (6)$$

Substituting equation (6) into equation (5) gives equation (7) as

$$Z_r(T) = \sum_{r=1}^{\infty} EXP \ \ln\left(\frac{K_B T}{D_0 6\pi\mu r^\varepsilon} \right) \qquad (7)$$

Thermodynamic properties such as Helmholtz free energy, $F(T)$, Entropy $S(T)$ Internal energy $U(T)$ and Specific heat $C_V(T)$ are obtained from the diffusional partition function as follows (Inyang *et al.,* 2022).

$$F(T) = -\frac{1}{T} \ln Z(T) \qquad (8)$$

$$S(T) = -K_B \frac{\partial F(T)}{\partial T} \qquad (9)$$

$$U(T) = -\frac{\partial}{\partial T} \ln Z(T) \qquad (10)$$

$$C_V(T) = K_B \frac{\partial U(T)}{\partial T} \qquad (11)$$

From equation (6) we have

$$D_0 = \frac{6\pi\mu r^\varepsilon}{K_B T} EXP^{\frac{E_r}{KT}} \qquad (12)$$

Substitute equation (12) into equation (3) gives,

$$E_r = KT \ln \frac{K_B D}{6\pi\mu r^\varepsilon} \frac{1}{BC} \qquad (13)$$

Using equations (1) and (13) the energy equation is obtained as,

$$E_r = KT \ln \frac{K_B D}{6\pi\mu r^\varepsilon} \frac{1}{B} \left[\frac{108D^2 n + 120Dn^2}{1620D^3 - 1935Dn + 204Dn^2 - 60n^3} \left(1 - \frac{n}{6D} r^2 \right) + \left(\frac{1}{r} - \frac{n}{2D} r \right) + \frac{90D^2 + 2Dn}{180D^2 - 15Dn + 6n^2} \left[r + \left(1 - \frac{n}{6D} r^2 \right) \right] \right]$$

4.0   Results and Discussion

We used the following parameters ($\varepsilon = 0.6, 0.7, 0.8, 0.9, 1.0$; $r = 1.0, 2.0, 3.0, 4.0, 5.0$; $n = 0.5$) and   (14)

$$K_B = 1.380650 X 10^{-23}; T = 500 C^{0}; \pi = 3.142$$

) to plot Figs 1 to 15. Fig. 1 shows the variation of Helmholtz free energy with temperature for Zn-Cu diffusion, with the radius of the diffusing entity as a variable. The plot indicates that as the radius of the diffusing species increases, the Helmholtz free energy also increases. This increase reaches a saturation point where further increases in the radius no longer affect the Helmholtz free energy, indicating temperature independence at this point. This behavior is consistent with the interpretation of Ikot *et al.* (2018), where thermal agitation due to the diffusing species' properties, such as viscosity and chemical nature, plays a significant role. Fig. 2 is a variation of the dependence of Helmholtz free energy on temperature with radius of diffusing entity varying for Iron-γ/Fe diffusion. From the plot a sharp saturation phase is seen along the energy and temperature axes and as the radius is raised the diffusing species experiences an exponential enhancement. This view is similar to that of Nitin *et al.* (2002). In Fig. 3, we present a similar analysis for Cu-Ni diffusion. Here, an exponential increase in Helmholtz free energy is observed as the radius of the diffusing species increases, followed by a saturation phase. After this saturation, the Helmholtz free energy continues to increase monotonically. This behavior aligns with the findings of Morozov and Skripkin (2011) and Edet *et al.* (2022), who attribute the observed patterns to the intrinsic characteristics of the diffusing species and the activation energy involved. Fig. 4 illustrates the variation of entropy with temperature for Cu-Cu diffusion. As the radius of the diffusing species increases, the plot shows a contraction along the temperature axis, indicating enhanced disorder at higher thermal energies. This behavior is attributed to the uniform and unrestricted diffusion of copper atoms into each other, leading to a steady increase in disorder, which aligns with Ravi and Paul's (2012) findings. Fig. 5 shifts focus to Cu-Al diffusion, where the entropy of the system increases exponentially after a saturation point along the temperature axis. A point of convergence is observed at very high thermal energies, further supporting the findings of Ikot *et al.* (2018). Fig. 6 explores the dependence of internal energy on temperature for Zn-Cu diffusion. The plot reveals a direct relationship between internal energy and temperature, with a monotonic increase in internal energy as the radius of the diffusing species increases. This observation suggests that the internal energy has a significant effect on the rate of diffusion, as supported by Laurila *et al.* (2010). Fig. 7 extends this analysis to Al-Al diffusion, where a thin saturation line is observed along the axes of internal energy and temperature. As the radius of the diffusing species increases, the internal energy also increases exponentially, reflecting the uniform nature of the diffusion process for identical atoms. This behavior is consistent with Ravi and Paul's (2012) interpretation. Fig. 8 depicts the behavior of internal energy in Fe-Fe diffusion (F.C.C. Iron). Similar to previous plots, saturation is observed along the internal energy and temperature axes. However, when the radius of the diffusing species is increased, the internal energy experiences a steady exponential increase. This increase is linked to the rise in kinetic energy and the energy stored in the chemical bonds between the molecules, a finding supported by Akira *et al.* (2018). Fig. 9 illustrates the dependence of heat capacity on temperature for Cu-Cu diffusion. The graph shows that heat capacity, being an extensive property, increases as more heat is required to raise the temperature of the system when the radius of the diffusing species is increased. Initially, a saturation point is

observed, but as the radius increases, the heat capacity rises exponentially. This result aligns with the views of Okorie *et al*. (2018). Fig. 10 presents the heat capacity variation for Al-Al diffusion. A slight saturation or contraction is observed along the temperature axis, indicating that little heat is needed to raise the temperature at low radii. As the radius increases, the heat capacity also increases monotonically, requiring more heat to maintain the diffusion process, similar to the observations by Takada *et al.* (2015). Fig. 11 concludes with the heat capacity variation for Mg-Al diffusion. Saturation is again observed along the heat capacity and temperature axes, but as the radius increases, the amount of heat required to achieve uniform diffusion increases monotonically. The plot shows an exponential increase in heat capacity with a convergence at the highest temperature, consistent with the findings of Inyang et al. (2021b). Fig. 12 is a plot of the dependence of entropy on temperature with the radius of the diffusing entity varying for Mg-Al diffusion. At elevated temperatures, there was a convergence and a corresponding increase in entropy; again, saturation was observed along the temperature axis. This concept is similar to that of Oyewumi *et al.* (2014). Fig. 13 shows the graphical dependence of internal energy on temperature with the radius of the diffusing entity varying for Cu-Ni diffusion. The graph shows a monotonical increase in internal energy when the radius of the diffusing entity was adjusted. This observation tallies with the work of researchers like Okorie *et al.* (2018). Fig. 14 depicts the dependence of internal energy on temperature with the radius of the diffusing entity varying for Fe diffusion. The internal energy increased monotonically with the variation of the radius of the diffusing entity. Internal energy is a function of temperature; as the thermal energy is raised, the molecules of the diffusing species become more mobile. This view is consistent with Inyang *et al.* (2024). Fig. 15 is a graph of the

dependence of heat capacity on temperature with the radius of the diffusing entity varying for Cu-Al diffusion. From the graph, when the radius of the diffusing entity was varied, there was a convergence at the highest temperature reached; thereafter, the heat capacity increased exponentially as the temperature also increased. This behavior is in agreement with the work of Inyang *et al.* (2021b).
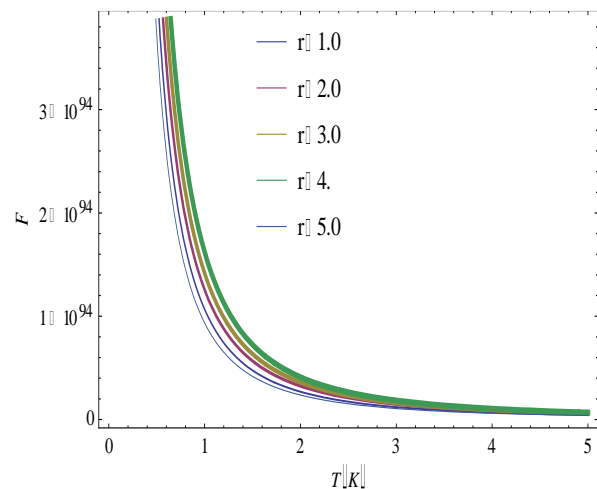

Fig. 1: Dependence of Helmholtz free energy on temperature with radius varying for Zn-Cu diffusion
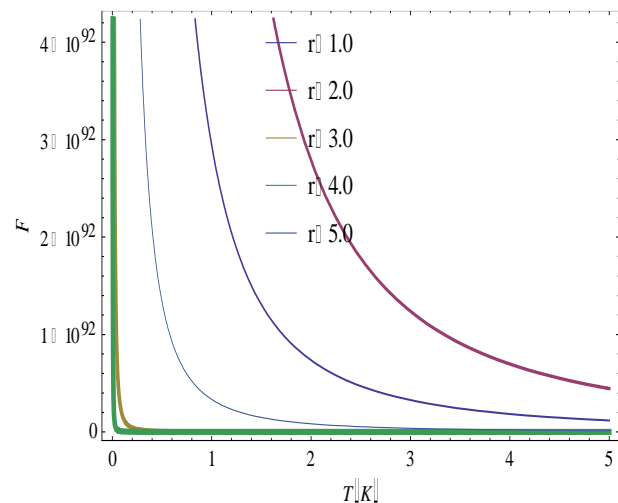

Fig. 2: Dependence of Helmholtz free energy on temperature with radius varying for Iron-γ/Fe diffusion (F.C.C. Iron)
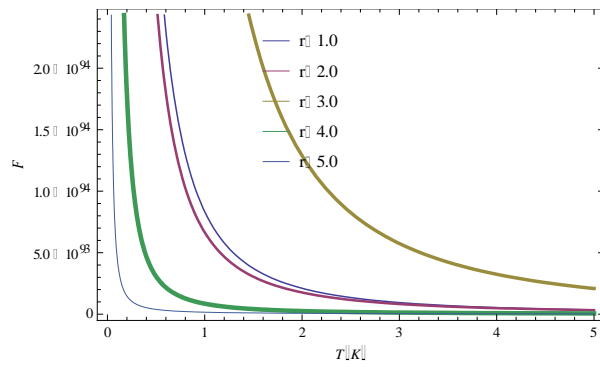
Fig. 3: Dependence of Helmholtz free energy on temperature with radius varying for Cu-Ni diffusion
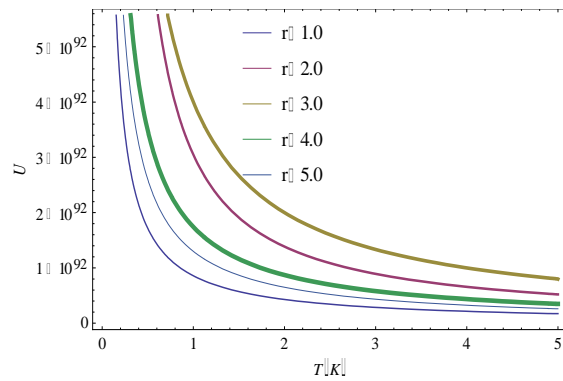
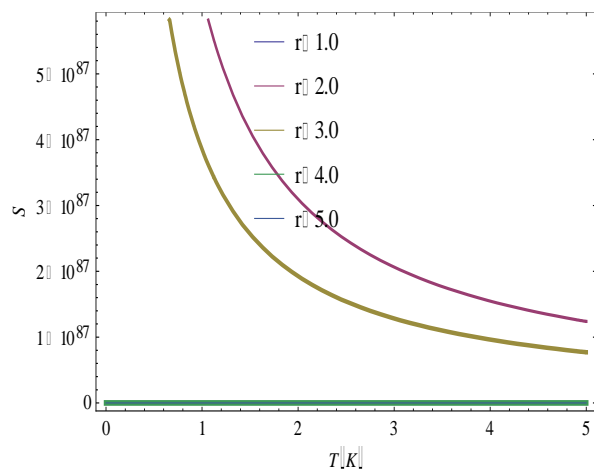**Fig. 6: Dependence of Internal energy on temperature with radius varying for Zn-Cu diffusion**

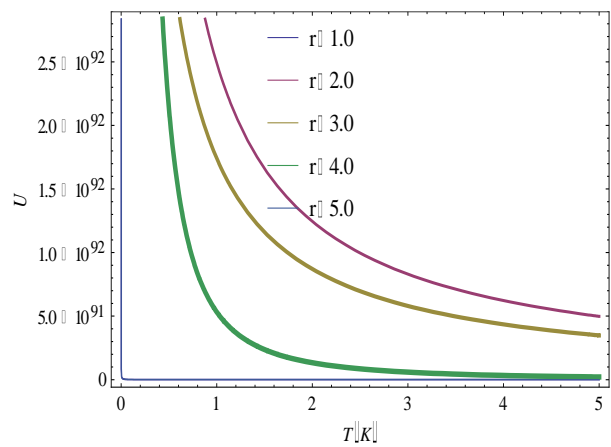**Fig. 4: Dependence of Entropy on temperature with radius varying for Cu - Cu diffusion**

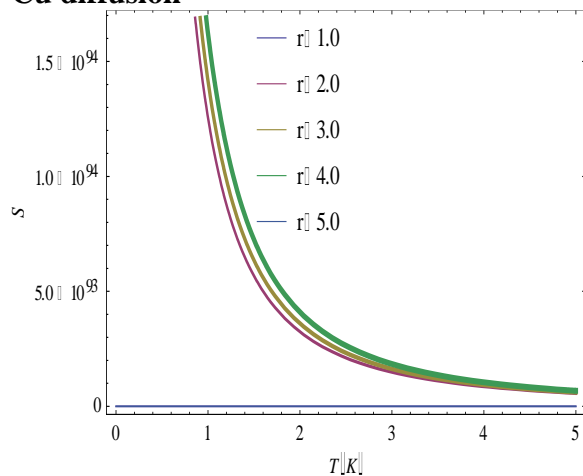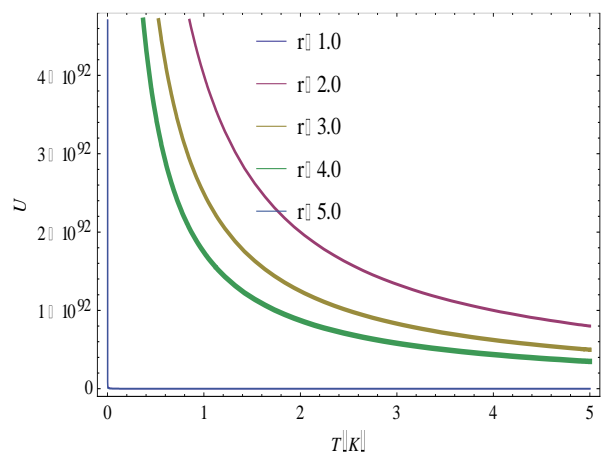**Fig. 7: Dependence of Internal energy on temperature with radius varying for Al-Al diffusion**

Fig. 5: Dependence of Entropy on temperature with radius varying for Cu-Al diffusion

Fig. 8: Dependence of Internal energy on temperature with radius varying for Iron-γ/Fe diffusion (F.C.C. Iron)
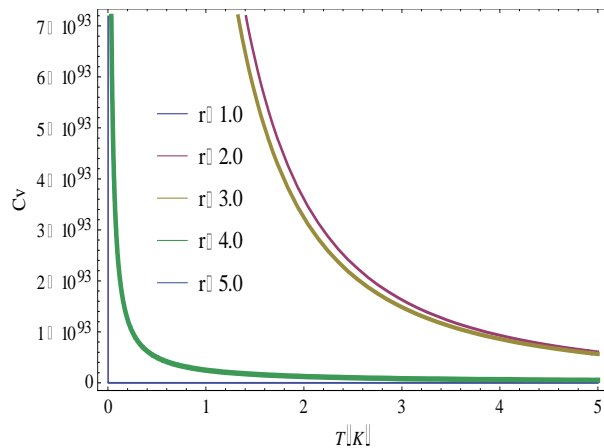
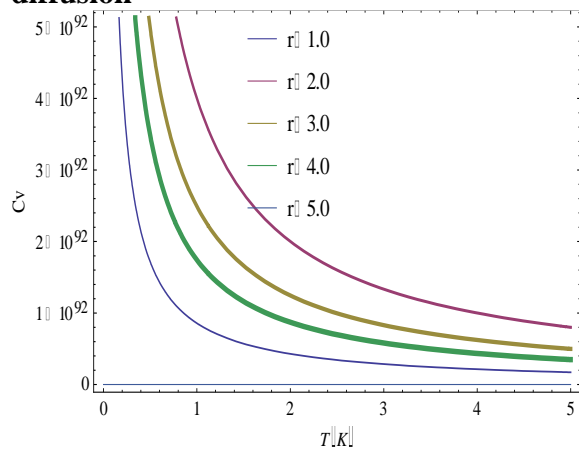**Fig. 9: Dependence of Heat capacity on temperature with radius varying for Cu-Cu diffusion**

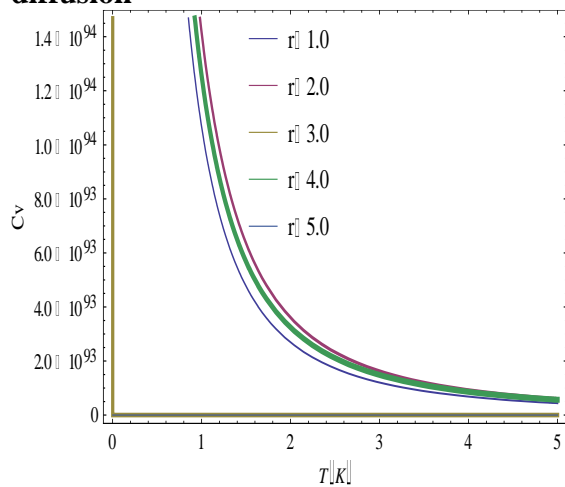**Fig. 10: Dependence of Heat capacity on temperature with radius varying for Al-Al diffusion**

Fig. 11: Dependence of Heat capacity on temperature with radius varying for Mg-Al diffusion
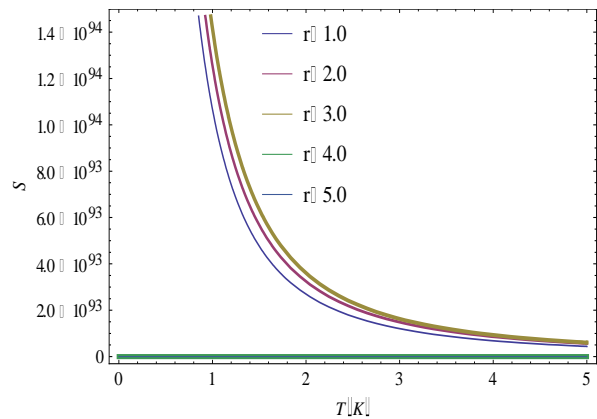

Fig. 12: Dependence of Entropy on temperature with radius varying for Mg-Al diffusion
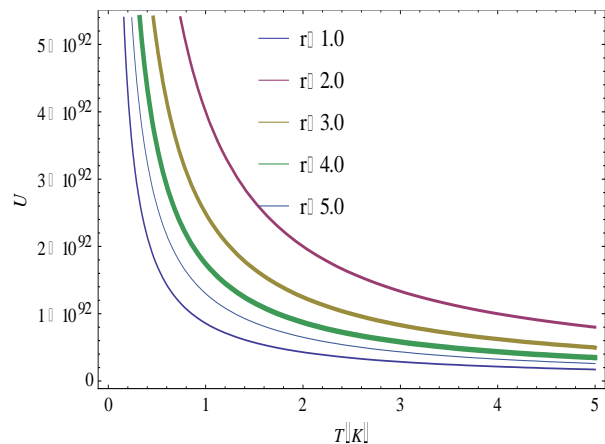

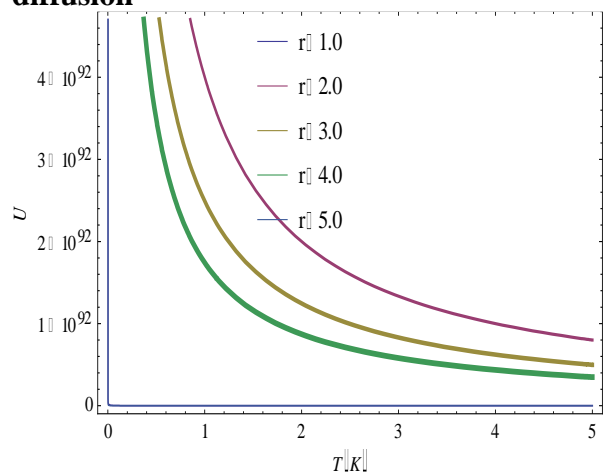**Fig. 13: Dependence of Internal energy on temperature with radius varying for Cu-Ni diffusion**

Fig. 14: Dependence of Internal energy on temperature with radius varying for Iron-α /Fe diffusion (B.C.C. Iron)
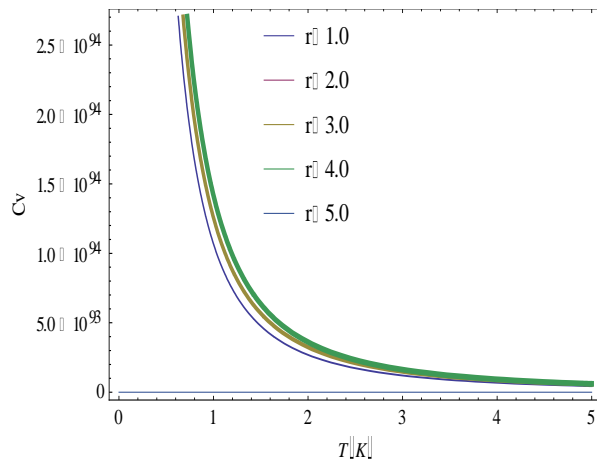
Fig. 15: Dependence of Heat capacity on temperature with radius varying for Cu-Al diffusion

5.0   Conclusions

In this study, the thermodynamic properties of the system were meticulously calculated using the Frobenius method and elegant solutions were derived from each plot. The rate of disorder increased as the thermal energy was adjusted upward, particularly in the case of entropy. Each property exhibited its distinct characteristics when subjected to varying conditions. This study provided a clear understanding of the relationship between classical mechanics and quantum mechanics, offering valuable insights into how these two fundamental frameworks interact under different thermodynamic scenarios.

6.0   References

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Compliance with Ethical Standards Declaration
Ethical Approval

Not Applicable

Competing interests

The authors declare that they have no known competing financial interests

Availability of data and materials

Data would be made available on request.

Authors Contribution

Akaezue, N. N, and Ngiangia, A. T., designed the study, performed the analytical analysis, and wrote the manuscript, Onyeaju, M. C., proofread and edited the manuscript. All authors read and approved the final manuscript.