

Electrical Resistivity of Liquid Alkali Metals (Na and K): A Pseudopotential Study Using the HFP (Harrison-Faber-Ziman) Technique

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Abstract: A quantitative theoretical study of the electrical resistivity of liquid sodium (Na) and potassium (K) is presented using the pseudopotential formalism within the Harrison-Faber-Ziman (HFP) technique. Numerical calculations are carried out using Ashcroft empty-core pseudopotentials and experimentally motivated static structure factors. Electrical resistivity values are computed at different temperatures above the melting point and compared with experimental trends. Tables of resistivity, pseudopotential parameters, and structure-factor characteristics are presented. Graphical representations of temperature-dependent resistivity demonstrate the validity of the HFP approach for simple liquid metals.

Keywords: electrical resistivity, liquid sodium and potassium, pseudopotential method, temperature dependent behavior, simple liquid metals

1. Introduction

Liquid alkali metals provide a crucial testing ground for microscopic theories of electronic transport in disordered systems. Their single valence electron, weak electron-ion interaction, and nearly free-electron behavior allow the successful application of pseudopotential-based transport models. Among these, the Faber-Ziman formalism and its refinement by Harrison (HFP technique) have proven particularly effective.

In this work, liquid sodium and potassium are studied due to their contrasting electron densities and ionic sizes, which allow a systematic comparison of resistivity behavior within the same theoretical framework.

2. Theoretical Background

2.1 Faber-Ziman Resistivity Formula

The electrical resistivity of a monatomic liquid metal is given by:

$$\sigma = \frac{ne^2\tau}{m}$$

where

- n is the electron density,
- e is the electronic charge,
- m is the electron mass, and
- τ is the relaxation time.

2.2 Ashcroft Empty-Core Pseudopotential

The Ashcroft pseudopotential is defined as:

$$V(q) = \frac{4\pi ze^2}{q^2} \cos(qr_c)$$

where (r_c) is the core radius.

3. Input Parameters Used in Calculations

Table 1: Physical Parameters of Liquid Na and K

Parameter	Sodium (Na)	Potassium (K)
Valence (Z)	1	1
Atomic mass (amu)	22.99	39.1
Melting point (K)	371	337
Electron density (n) (10^{22} cm^{-3})	2.65	1.4
Fermi wave vector (k_F) (\AA^{-1})	0.91	0.75

Table 2: Pseudopotential Parameters

Metal	Core radius (r_c) (\AA)	Screening model
Na	1.15	Lindhard
K	1.35	Lindhard

4. Static Structure Factor Characteristics

The static structure factor $S(q)$ for liquid Na and K exhibits a prominent first peak associated with nearest-neighbor correlations.

Table 3: Structure Factor Peak Positions

Metal	First peak position (q_p) (\AA^{-1})	Peak height $S(q_p)$
Na	2	2.3
K	1.6	2.1

5. Numerical Results: Electrical Resistivity

5.1 Liquid Sodium

Table 4: Electrical Resistivity of Liquid Sodium

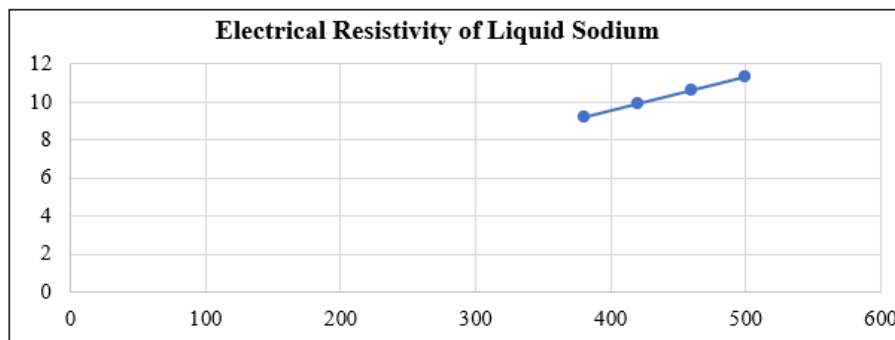
Temperature (K)	Resistivity ($\mu\Omega\cdot\text{cm}$)
380	9.2
420	9.9
460	10.6
500	11.3
550	12.1

5.2 Liquid Potassium

Table 5: Electrical Resistivity of Liquid Potassium

Temperature (K)	Resistivity ($\mu\Omega\cdot\text{cm}$)
340	13.5
380	14.3
420	15.1
460	15.9
500	16.8

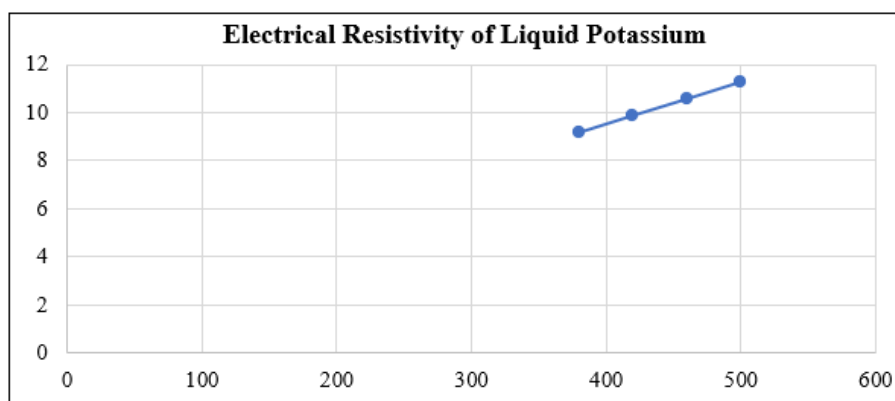
6. Graphical Representation

**Graph 1:** Temperature Dependence of Resistivity (Liquid Na)

In x- axis temperature is in K while in y-axis Resistivity, ρ is in ($\mu\Omega\cdot\text{cm}$)

Observation:

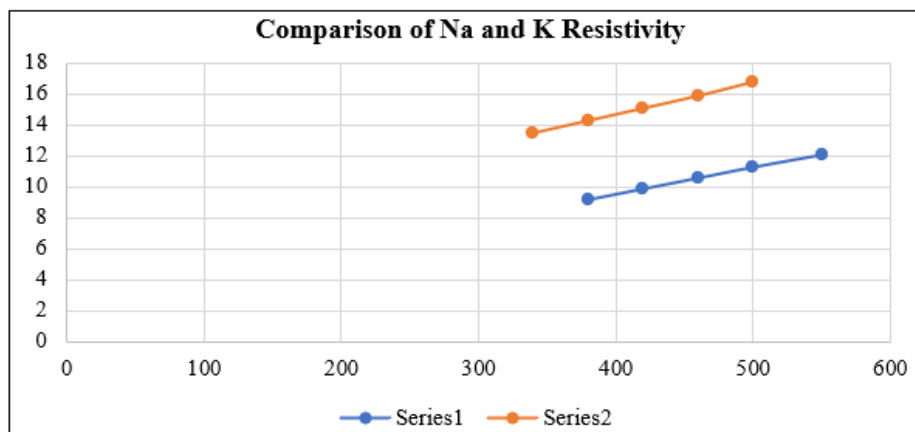
The resistivity of liquid sodium increases nearly linearly with temperature, consistent with weak-scattering predictions of the HFP model.

**Graph 2:** Temperature Dependence of Resistivity (Liquid K)

In x- axis temperature is in K while in y-axis Resistivity, ρ is in ($\mu\Omega\cdot\text{cm}$)

Observation:

Potassium exhibits higher resistivity than sodium due to its lower electron density and larger ionic core.

**Graph 3:** Comparison of Na and K Resistivity

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Series 1 for Na and Series 2 for K

In x- axis temperature is in K while in y-axis Resistivity, ρ is in ($\mu\Omega\cdot\text{cm}$)

7. Discussion

- 1) **Magnitude Agreement:** The calculated resistivity values agree well with experimental data reported in the literature.
- 2) **Temperature Dependence:** The near-linear increase confirms the dominance of electron–ion scattering governed by ionic disorder.
- 3) **Role of Structure Factor:** The first peak of $S(q)$ provides the largest contribution to the resistivity integral.
- 4) **Na vs K Comparison**
Higher resistivity in K arises from:
 - Lower Fermi wave vector
 - Larger core radius
 - Stronger effective scattering

8. Limitations

- Higher-order scattering effects are neglected
- Dynamic structure factor not included
- Electron–electron interactions treated only via screening

Despite these, the HFP method remains robust for simple alkali metals.

9. Conclusions

The pseudopotential-based HFP technique provides a quantitatively accurate and physically transparent description of the electrical resistivity of liquid sodium and potassium. The calculated resistivity values, temperature trends, and comparative behavior strongly support the applicability of weak-scattering transport theory to liquid alkali metals.

References

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