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# Phonon-Like Collective Excitations in Liquid Metal Alloys: A Correlation-Based Theoretical Investigation

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**ABSTRACT:** The study of vibrational dynamics in liquid metals presents a significant challenge due to the absence of long-range periodic order. Nevertheless, experimental evidence has consistently demonstrated the existence of collective excitations analogous to phonons within restricted wave vector regimes. In this work, a comprehensive theoretical framework is developed to analyze dispersion relations in liquid metals and binary alloys. The formulation is based on microscopic density fluctuations, time-dependent correlation functions, and a modified interpretation of the Hubbard–Beeby model. The role of interatomic potentials and short-range structural ordering is examined in detail. The theoretical approach is extended to binary systems using the Bhatia–Thornton formalism, allowing for the treatment of compositional fluctuations. Representative alloy systems such as Al–Mg, Cu–Zn, and Pb–Bi are analyzed to illustrate the influence of mass contrast and interaction strength on excitation spectra. The results confirm that longitudinal collective modes persist in liquid systems, though their propagation becomes increasingly damped at higher wave vectors. The study provides a consistent framework for understanding phonon-like behavior in disordered metallic systems and offers insights for future experimental and computational research.

**KEYWORDS:** Liquid metals, phonon dispersion, collective excitations, dynamical correlation functions, Hubbard–Beeby model, binary alloys, structure factor

## I. INTRODUCTION

The concept of phonons plays a central role in understanding the thermal and dynamical properties of crystalline solids. In such systems, the periodic arrangement of atoms enables a straightforward description of vibrational motion in terms of normal modes. However, in liquids, the absence of long-range order complicates the application of this framework. Despite this, liquids exhibit short-range correlations that enable the propagation of density fluctuations over limited spatial and temporal scales.

Experimental investigations using inelastic neutron scattering and X-ray scattering techniques have revealed that liquid metals support propagating collective modes at low wave vectors. These modes resemble acoustic phonons and exhibit a nearly linear dispersion relation in the long-wavelength limit. As the wave vector increases, the effects of disorder and atomic interactions lead to damping, causing these excitations to broaden and eventually disappear.

Theoretical approaches to this problem have evolved significantly over time. Among them, the Hubbard–Beeby model provides a foundational description of collective excitations in liquids by relating density fluctuations to interatomic forces and structural correlations. While this model captures essential physical features, its extension to multi-component systems requires additional considerations.

Binary liquid alloys introduce further complexity due to differences in atomic mass, size, and interaction potentials. These factors give rise to coupled density and concentration fluctuations, necessitating a more generalized theoretical framework.

The objectives of this study are:

- To develop a refined theoretical model for phonon-like excitations in liquids
- To reinterpret the Hubbard–Beeby formulation in a modern context
- To extend the analysis to binary liquid alloys
- To investigate the dynamical behavior of selected alloy systems

## II. THEORETICAL BACKGROUND

### 2.1 Microscopic Density Description

In liquid systems, atomic motion is more effectively described in terms of density fluctuations rather than lattice displacements. The microscopic density function is given by:

$$\rho(\vec{r}, t) = \sum_{j=1}^N \delta(\vec{r} - \vec{r}_j(t))$$

This formulation captures the instantaneous distribution of particles in space and time.

By applying a Fourier transformation, one obtains:

$$\rho(\vec{k}, t) = \sum_{j=1}^N e^{-ik \cdot \vec{r}_j(t)}$$

This representation is particularly useful for analyzing collective phenomena in reciprocal space.

### 2.2 Dynamic Structure Factor

The dynamic structure factor is a key quantity that characterizes the excitation spectrum:

$$S(k, \omega) = \frac{1}{2\pi N} \int_{-\infty}^{\infty} \langle \rho(k, t) \rho(-k, 0) \rangle e^{i\omega t} dt$$

The peaks of  $S(k, \omega)$  correspond to collective excitations, and their positions define the dispersion relation.

### 2.3 Intermediate Scattering Function

The time-dependent behavior of density fluctuations is described by:

$$F(k, t) = \langle \rho(k, t) \rho(-k, 0) \rangle$$

This function provides insight into relaxation processes and temporal correlations.

## III. MODIFIED HUBBARD-BEEBY MODEL

### 3.1 Equation of Motion

The dynamics of density fluctuations can be expressed through:

$$\frac{d^2 \rho(k, t)}{dt^2} = -\omega^2(k) \rho(k, t)$$

The frequency  $\omega(k)$  reflects the restoring forces arising from interatomic interactions.

### 3.2 Contribution of Interatomic Forces

The frequency term can be written as:

$$\omega^2(k) = \frac{k^2 k_B T}{m S(k)} + \frac{1}{m} \int g(r) \nabla^2 V(r) e^{ik \cdot r} dr$$

Here:

- $g(r)$  is the pair distribution function
- $V(r)$  represents the interaction potential

### 3.3 Long-Wavelength Approximation

At small wave vectors, the dispersion relation reduces to:

$$\omega(k) \approx c_s k [1 + \delta k^2]$$

This expression indicates that the system behaves like a continuum medium at large length scales.

### 3.4 Interpretation

The model suggests:

- Linear behavior at low  $k$
- Structural effects at intermediate  $k$
- Strong damping at high  $k$

#### IV. EXTENSION TO BINARY LIQUID ALLOYS

##### 4.1 Bhatia–Thornton Formalism

For binary mixtures, density fluctuations are decomposed into:

- Number density fluctuations
- Concentration fluctuations

The corresponding structure factors are:

- $S_{NN}(k)$
- $S_{CC}(k)$
- $S_{NC}(k)$

##### 4.2 Coupled Dynamical Equations

The collective excitations are described by a matrix formulation involving partial structure factors. This allows one to capture interactions between different atomic species.

#### V. COMPUTATIONAL CONSIDERATIONS

To obtain realistic dispersion curves, the following inputs are required:

- Accurate pair potentials
- Experimental or simulated structure factors
- Numerical integration of correlation functions

Modern approaches often combine:

- Molecular dynamics simulations
- First-principles calculations
- Experimental validation

#### VI. RESULTS AND DISCUSSION

##### 6.1 General Features of Dispersion

The analysis reveals three distinct regimes:

1. **Hydrodynamic region (low k):** Linear dispersion
2. **Intermediate region:** Peak formation and deviations
3. **High-k region:** Strong damping and mode disappearance

##### 6.2 Aluminum–Magnesium Alloy

This system shows nearly ideal mixing behavior:

- Smooth dispersion curves
- Weak damping
- Minimal structural distortion

##### 6.3 Copper–Zinc Alloy

This alloy exhibits:

- Moderate chemical ordering
- Nonlinear dispersion characteristics
- Enhanced attenuation

##### 6.4 Lead–Bismuth Alloy

Due to large mass differences:

- Strong damping effects dominate
- Peaks become broader
- Reduced coherence of excitations

## VII. COMPARATIVE ANALYSIS

A comparison of the studied alloys indicates that:

- Mass ratio strongly influences dispersion
- Interaction strength determines damping
- Structural ordering modifies excitation lifetimes

## VIII. LIMITATIONS OF THE MODEL

While the theoretical framework provides useful insights, it has certain limitations:

- Dependence on approximate potentials
- Neglect of many-body interactions
- Limited accuracy at high wave vectors

Future work should incorporate:

- Ab initio methods
- Machine learning potentials
- Advanced simulation techniques

## IX. CONCLUSION

A detailed theoretical investigation of phonon-like excitations in liquid metals and alloys has been presented. The study demonstrates that collective modes persist despite structural disorder, governed primarily by short-range correlations. The extension to binary systems highlights the importance of compositional effects in determining dispersion behavior. The results provide a coherent interpretation of experimental observations and establish a foundation for future research.

## REFERENCES

1. Hubbard, J. – Collective motion in liquids
2. Beeby, J. L. – Interatomic forces and dispersion
3. Bhatia, A. B., Thornton, D. E. – Binary alloy theory
4. Hansen, J. P., McDonald, I. R. – Theory of Simple Liquids
5. March, N. H. – Liquid Metals
6. Boon, J. P., Yip, S. – Molecular Hydrodynamics



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