Journal of
Physics and Chemistry of Materials
Vol.**12**, Issue.**1**, pp.**01-07**, March **2025**
E-ISSN: 2348-6341
Available online at: www.isroset.org

Research Article

Theory for Dynamical Structure Factors of Liquid Potassium at Melting Temperature

Grima Dhingra[1]

[1]Dept. of Physics, Maharshi Dayanand University, Rohtak, Haryana, India

**Corresponding Author:*

Received: 22/Dec/2024; **Accepted**: 14/Feb/2025; **Published**: 31/Mar/2025. | **DOI**: https://doi.org/10.26438/jpcm/v12i1.17

Abstract— A microscopic theoretical approach is employed to calculate the detailed dynamical structure factors of an interacting fluid of potassium atoms at its melting temperature. The theoretical investigation is carried out at 338 K, where 0.845 grams of the interacting particles occupy one cubic centimetres of the fluid. The calculations are performed over a range of κ (wave vector): 0.3 $Å^{-1}$ to 3.0 $Å^{-1}$. This theoretical approach utilizes the inter-particle interactions present among the constituent particles of the liquid to calculate various dynamical quantities including the dynamical structure factor and the current-current correlation function. The predicted dynamical functions in turn allow for the determination of key transport properties; diffusion coefficient, and longitudinal viscosity and other significant properties, such as collective mode frequencies and the sound velocity. These properties are reported for the entire κ–range. The modified microscopic theory, therefore, is emerged as an inclusive method, for calculating the complete dynamics of liquid potassium at the melting temperature by incorporating inter-particle interactions.

Keywords— Equilibrium Dynamics, Dynamical structure factor, Inter-particle interaction, Current-current correlation function, Diffusion coefficient, Modified microscopic theory

1. Introduction

Various theories [1-4] describing the complicated dynamics of the interacting fluids, have been proposed wherein the degree of correlations among its particles can range from strongly to weakly correlate and are characterized by the presence of single and collective particle motion. At the same time, there are various theories to [5,6] explain transport phenomena and to quantitatively determine transport coefficients such as diffusion coefficient in liquids and gases. However, these coefficients are rarely gauged in terms of the interactions and correlations present between the particles of a fluid. Such an endeavour has been made in this current study by applying the modified microscopic theory for the purpose of describing the complete dynamics along with one of the transport coefficients, the diffusion coefficient of liquid potassium at 338K, just at its melting point (336 K). The computations have been performed for a wider wave vector range of 0.3 $Å^{-1} \leq \boldsymbol{\kappa} \leq 3.0$ $Å^{-1}$. The fluid under investigation is a system of moving potassium atoms of approximately 1.27 × 10^{22} particles present per cubic centimetre. This is apparent to understand that constituent particles of liquid potassium (K) at the melting temperature are interacting with high energy. This makes the fluid potassium to be a vastly interactive and strongly correlated system. Therefore, application of the modified microscopic theory of such a classical fluid system to describe its dynamics, is well-founded.

Studying the collective dynamics of fluids has always been a challenging task. A theorist may need pure coherent scattering cross sections measured from experiments to successfully validate their outcomes. Experimental methods, on the other hand, such as inelastic X-ray scattering and thermal neutron inelastic scattering, are generally used to study the communal motions of interacting particles but are subject to definite restrictions. The previously used method of scattering by neutrons (INS) results in a mixture of cross-sections from incoherent scattering and coherent scattering in nearly equivalent amounts [7, 8], making it tough to extract the coherent structural information from the spectra. From the inelastic scattering of X-rays, in contrast, when conducted at the high-resolution synchrotron radiation sources [9], can provide data which is purely coherent. Recent experimental IXS coherent spectral line shape data for liquid potassium at 343 K, within a wave vector range of 0.9–17.0 nm^{-1}, has been reported by Monaco et al. [10]. The temperature for this study from scattering of X-rays is, however, above the melting temperature. The coherent spectral line-shapes for liquid potassium at the melting temperature have not been reported by the IXS experiment, and hence, this necessitates the theoretical evaluation for the detailed dynamical structures to explore the complete dynamics of given fluid, liquid potassium.

This paper is structured into five different sectors: including, Introduction, Related work, Mathematical Formalism, Results and Discussion, and Conclusion. In the first section a layout of introduction to the research problem and literature review has been provided. In section II outlines the basic propositions and related theoretical framework employed in this study. Layout of mathematical formalism containing mathematical expressions for various physical quantities in relation to the present microscopic theory are presented in section III. In section IV presentation of computed results in the case of fluid under study has been made and is followed by an in-depth discussion. Finally, Section V summarizes the conclusions derived from the theoretical outcomes.

2. Related Work

In the present work, the entire dynamics of liquid potassium along with the dynamical structure factor are deduced from an approach that relies on the microscopic dynamics of the liquid. By employing apt averages over time spans of the solved classical equations of motion of moving particles, the current theory examines the reaction of an interacting, correlated fluid to invading radiation (X-rays or neutrons) [11] and hence, exhibit time-related disorders. The well-known, Fluctuation-Dissipation Theorem establishes a connection of the imaginary part of the complex function obtained from the density response function when Fourier transformed in space and time, to the dynamical structure factor. Though the motion of distinct particles is correlated, these correlations were neglected in the previous microscopic theory [11]. Such correlations are incorporated into the present form of the theory by defining the characteristic relaxation time [12], which is further influenced by various substantial properties of the system, including the static structure factor, diffusion coefficient, interaction potential, mass, temperature and density.

In this theoretical approach, the diffusion coefficient is acquiring a specific value for a given wave vector. The theory is further modified by making diffusion coefficient frequency dependant so as to obtain agreement to experimental values leading to realistic description of the intermediate scattering function without entertaining arbitrary parameters.

Collective dynamics of a number of liquids has been explained previously applying this form of modified microscopic theory [13-17]. In the present work, this approach is implemented for the determination of the collective dynamics of liquid potassium.

3. Mathematical Formalism

As described in the prior section, connection between the dynamical structure factor and the imaginary part of the Fourier transform of the density-2 response function is established through the Fluctuation-Dissipation Theorem and is given as:

$$S(\vec{\kappa},\omega) = -\frac{k_B T}{\pi\rho_0}\,\frac{\chi''(\vec{\kappa},\omega)}{\omega}$$

Here, $\chi(\vec{\kappa},\omega)$ is a complex function obtained when the density-2 response function is Fourier transformed and $\chi''(\vec{\kappa},\omega)$ is the imaginary part of the $\chi(\vec{\kappa},\omega)$. *T*, here, is the temperature, and ρ_o denotes the number density of particles.

The density-2 response function characterizes the behaviour of a liquid when subjected to a weak external probe, causing space-time dependent fluctuations in the equilibrium density. Microscopic theory provides a method to derive this function $\chi(\vec{\kappa},\omega)$ by solving the micro-dynamics of the liquid. The trajectories of moving particles are obtained by solving the classical equations of motion, and their history averages lead to the calculation of complex space-time dependent correlation functions. In earlier microscopic theories, time-dependent correlations were ignored, resulting in dynamical structure factors that deviated significantly from experimentally observed spectral line shapes. To address this, a characteristic relaxation time was introduced to satisfy the zeroth sum rule. Applying this modified microscopic theory yielded significantly improved results for the dynamical structure factors of various liquids [18-22].

The dynamical structure factor in this form of theory acquires the following form:

$$S(k,\omega) = \frac{k^2}{\pi m\beta}\left\{\left[1+\omega_k^{\,2}\,\frac{(\beta''+\gamma)^2-\omega^2}{\left[(\beta''+\gamma)^2+\omega^2\right]^2}\right]\frac{2\beta''}{\left(\beta''^2+\omega^2\right)^2} - \omega_k^{\,2}\,\frac{\left(\beta''^2-\omega^2\right)}{\left(\beta''^2+\omega^2\right)^2}\,\frac{2(\beta''+\gamma)}{\left[(\beta''+\gamma)^2+\omega^2\right]^2}\right\}$$

$$x\left\{\left[1+\omega_k^{\,2}\,\frac{(\beta''+\gamma)^2-\omega^2}{\left[(\beta''+\gamma)^2+\omega^2\right]^2}\right]^2 + \left[\omega_k^{\,2}\,\frac{2\omega(\beta''+\gamma)}{\left[(\beta''+\gamma)^2+\omega^2\right]^2}\right]^2\right\}^{-1} \tag{1}$$

Here, in the expression (1), $\beta'' = D_{eff}\ \kappa^2$, D_{eff} is diffusion coefficient turns to be frequency dependant.
$\beta = (k_BT)^{-1}$ and, $\Upsilon = \tau(\kappa)^{-1}$,
The relaxation time $\tau(\kappa)^{-}$is defined as follows:

$$[\tau(\kappa)]^{-1} = \frac{\omega_\kappa}{\left[\left(\kappa^2/m\beta S(\kappa)\beta'^2\right)-1\right]^{1/2}} - \beta' \tag{2}$$

Here, β' = D κ^2, with D being κ-dependant diffusion coefficient.

m is the atomic mass and $S(\kappa)$ is the static structure factor.

$S(\kappa)$ can be obtained from the Fourier transform of the static pair correlation function, $g(r)$ from the following expression:

$$S(\kappa) = 1 + 4\pi\rho_0 \int_0^\infty r^2 (g(r)-1) \frac{\sin \kappa r}{\kappa r} dr \tag{3}$$

Also,

$$\omega_\kappa{}^2 = \omega_E{}^2 \left[1 - \frac{3\sin \kappa r_0}{\kappa r_0} - \frac{6\cos \kappa r_0}{(\kappa r_0)^2} + \frac{6\sin \kappa r_0}{(\kappa r_0)^3}\right] \tag{4}$$

Where, ω_E, is the elastic frequency given as follows:

$$\omega_E{}^2 = \frac{4\pi\rho_0}{3m} \int \left(\frac{\partial^2 V}{\partial r^2} + \frac{2}{r}\frac{\partial V}{\partial r}\right) g(r) r^2 dr \tag{5}$$

Here, $\mathrm{V}(r)$ is the inter-atomic potential.

r_0 occurred in the expression (4) is obtained on applying following approximation:

$$\frac{\partial^2 V}{\partial z^2} g(r) = A\delta(r - r_0) \tag{6}$$

The peak of the delta function is $r = r_0$ and z is the space coordinate.

$C(\kappa, \omega)$ is the current-current correlation function and is given by the following expression:

$$C(\kappa, \omega) = \frac{\omega^2}{\kappa^2} S(\kappa, \omega) \tag{7}$$

4. Results and Discussion

As is discussed in the preceding section, the determination of the detailed dynamical structure factors requires the entailment primarily of the inter-particle interaction potential and also the pair distribution function, g(r). The framework of microscopic theory evolves from the interaction potential with which the particles of given fluid interact. For the current work, the interaction potential for liquid potassium proposed by J.M.G. Miranda [23] has been used. While carrying molecular dynamics, four different potential forms for liquid potassium, evolved from the pseudopotential by Ashcroft and also dielectric function, have been considered. The first form of interaction potential is devoid of usual Born-Mayer term for interaction at the given temperature potentials, whereas the other two forms have included the BM term with the effective ionic radii to evolve the dynamical properties. The fourth proposed form of interaction potential focused on the agreement between experimental and calculated results and is the one that has been observed to accentuate on the coupling of the longitudinal modes due to the softening of the repulsive core, when the Born-Mayer term is incorporated in. This form of interaction potential, which has successfully regenerated the static structure factor for liquid potassium reported from X-ray diffraction study [24] and hence, has been chosen here for further computations. Another noticeable form of inter-particle interaction potential for the fluid, reported by Brettonet and Jakse [25], has also been observed to yield the static structure factor and hence, the static pair correlation function with accordance to the experimentally measured static structure factor, by Hujiben et al. [26]. However, the former appears to be in a better agreement to X-ray diffraction study and, hence, has been implied in the current work out.

On substituting the empirical form of this interaction potential, along with the static pair correlation function g(r), in expression (5), Einstein frequency, ω_E, has been evaluated. From the expression (6) the peak position of the delta function, r_o has been calculated. These two entities ω_E and r_o for liquid K at 338 K turn out to be 1.342 × 10^{13} s^{-1} and 4.4 Å, respectively, and on substituting into expression (4) yielded κ-dependant frequency, ω_κ. The static pair correlation used here is that obtained from the experimental static structure factor (expression (3)), when Fourier transformed. The values for these quantities have been further used in the expression (2) for the computation of the relaxation time. This single characteristic relaxation time, τ(κ), is incorporated into the modified microscopic theory to account for the distinct particle correlations. It reflects the evolution with time of distinct properties, such as particle positions or densities. In quintessence, the wave-vector dependent evolution of the system over a timescale to attain equilibrium after a perturbation is described.

In expression (2), appeared a parameter, the diffusion coefficient, D which is included to ensure the fulfilment of the zeroth sum rule for a given wave-vector, κ. The zeroth sum rule serves as a normalization condition, ensuring that the dynamical structure factors are correctly formed across all ω ranges. The modified microscopic theory, therefore, adheres to all sum rules for liquids. With the relaxation time and diffusion coefficient, the detailed dynamical structure factors, S(\κ,ω), have then been calculated. The detailed structure factors describe the occurrence of fluctuations in space as well as over time and hence, can provide essential insight into the dynamic conduct a system carries. They are deduced using expression (1), that links S(κ,ω) and τ(κ) through the diffusion coefficient, *D*.

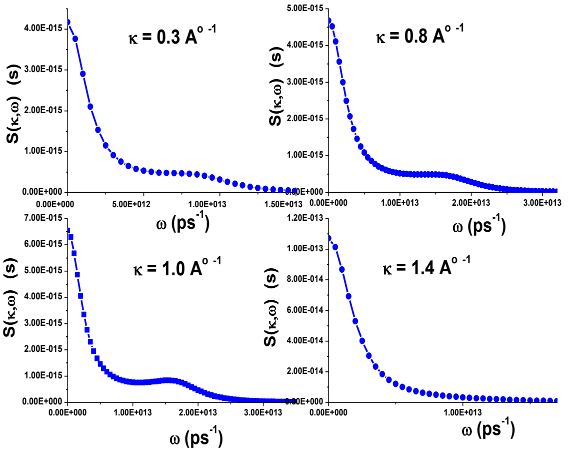

Figure 1: Dynamical structure factor, $S(\kappa,\omega)$ of liquid potassium at 338 K versus frequency, ω: (—●—) present theory at κ =0.3 Å^{-1} , κ = 0.8 Å^{-1} , κ = 1.0 Å^{-1} and κ =1.4 Å^{-1}.

The dynamical structure factors have been calculated for eight values of the wave-vector in the entire range of 0.3 Å^{-1} - 3.0 Å^{-1}. The obtained results that show the variation of the dynamical structure factors with frequency, ω, have been offered in Figure 1 for κ = 0.3 Å^{-1}; κ = 0.8 Å^{-1}; κ = 1.0 Å^{-1} and κ = 1.4 Å^{-1}: denoted by solid-circle curves (− ● −). Similar variation of dynamical structure factors have been shown in Figure 2 for κ = 1.65 Å^{-1}; κ = 2.0 Å^{-1}; κ = 2.5 Å^{-1} and κ = 3.0 Å^{-1}: with solid-circle curves, (− ● −). In these calculations, the effective diffusion coefficient turns out to be κ-dependant as given in expression (2). As can be seen from the figures, at smaller values of wave-vectors, κ, up to κ= 1.0 Å^{-1}., the three peak structures along with the appearance of Brillouin peaks are exhibited. On increasing the wave-vector values, for κ > 1.0 Å^{-1}, much damper line shapes for the dynamical structure factors with the absence of the Brillouin peaks, are quoted. For the sake of comparison, the calculated data is compared with results from an IXS study for liquid potassium [10], though performed at an elevated temperature of 343 K, for two different values of wave-vector κ, κ = 0.3 Å^{-1} and κ = 1.0 Å^{-1}. The corresponding results from the experimental study (though at a different temperature) have been shown in Figure 3 with solid-square curves (−■−) and results from the present study have been drawn with a solid-circle curve (−●−), for both κ values. The comparison reveals that the structures obtained from IXS for the higher temperature at both wave vector values, have turned rather well defined, sharper and are recognised with prominent Brillouin peaks. Moreover, the peak positions have been appeared to shift towards the smaller frequencies. The difference in the outcomes from the two considerations can be accredited to the difference in temperatures.

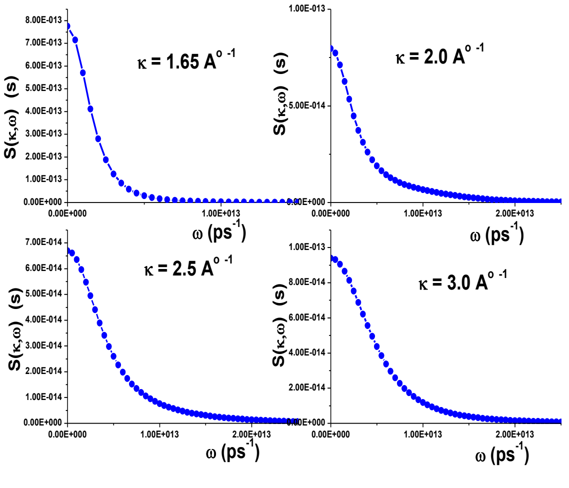

Figure 2: Dynamical structure factor, $S(\kappa,\omega)$ of liquid potassium at 338 K versus frequency, ω: (—●—) present theory at κ =1.65 Å^{-1} , κ = 2.0 Å^{-1} , κ = 2.5 Å^{-1} and κ =3.0 Å^{-1}.

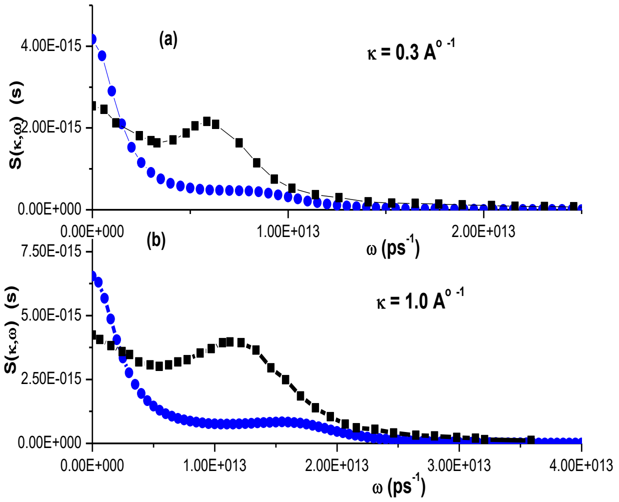

Figure 3(a): Dynamical structure factor, $S(\kappa,\omega)$ versus frequency, ω, of liquid potassium at 338 K at κ = 0.3 Å^{-1}: (—●—) present theory; (—■—) experimental results (ref. [10]).

Figure 3(b): Dynamical structure factor, $S(\kappa,\omega)$ versus frequency, ω, of liquid potassium at 338 K at κ = 1.0 Å^{-1}: (—●—) present theory; (—■—) experimental results (ref. [10]).

The computed dynamical structure factors when entailed in the expression (7) now, to provide the single-peaked functions, the current-2 correlation functions. Figure 4 displays the computed results of *C*(κ,ω) the current-2 correlation function, derived from the dynamical structure factors using expression (7), for all wave-vector values. The variation of C(κ,ω) with ω has been shown with: (———) κ = 0.3 Å^{-1}; (- - - - -) κ = 0.8 Å^{-1}; (− · − · −) κ = 1.0 Å^{-1};

(− · · −) κ = 1.4 Å^{-1}; (••••••••••) κ = 1.65 Å^{-1}; (──×──) κ = 2.0 Å^{-1}; (—▲—) κ = 2.5 Å^{-1} and (—Δ—) κ = 3.0 Å^{-1}. The positions of the peaks of current-2 correlation functions correspond to the collective mode frequencies at a given value of κ. The collective mode frequency for a given wave vector, can also be depicted from the dynamical structure factors as the position of the Brillouin peaks in the detailed structures.

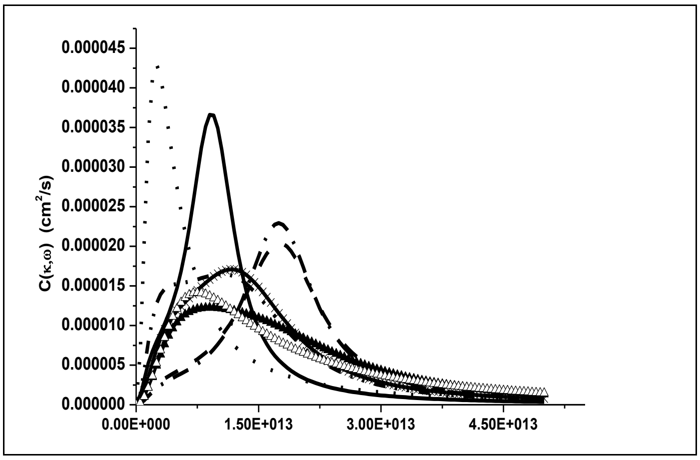

Figure 4: Variation of the Current-2 correlation functions, calculated from the dynamical structure factors of Fig. 1 and Fig. 2 for different values of wave –vector, with frequency ω: (────) κ = 0.3 Å^{-1}; (- - - - -) κ = 0.8 Å^{-1}; (− · − · −) κ = 1.0 Å^{-1}; (− · · · −) κ = 1.4 Å^{-1}; (••••••••••), κ = 1.65 Å^{-1}; (──×──) κ = 2.0 Å^{-1}; (—▲—) κ = 2.5 Å^{-1} and (—Δ—) κ = 3.0 Å^{-1}.

However, the wave vectors, specifically higher κ, for which dynamical structures are damped and side peaks are not visible, the collective modes can be quoted from the current-2 correlation functions, at the position where peak of the function lies.

The collective mode frequencies, $\omega_{p,}$ deduced from the current-2 correlation functions, have been plotted in Figure 5(a), as their variation against κ : with solid circles (-●-), ω_p. The frequencies of collective excitations shown in figure 5(a) correspond to the peak position of C(κ,ω) of figure 4 and their variation with κ yields the dispersion relation for the liquid. As can be seen in the figure, the collective mode frequencies increase with an increase in the wave-vector to a maximum at nearly κ = 0.8 Å^{-1} , decreases with the further increase in wave vector up to a minimum at κ =1.65 Å^{-1}, wave-vector corresponding to peak position of the static structure factor and increases thereafter with further increase in the wave-vector, κ . A secondary peak at κ = 2.0 Å^{-1} has also appeared in the dispersion curve. This pattern reflects the characteristic drift for the variation of the dispersion relation. The theory incorporates correlations among different particles by defining characteristic relaxation time through the diffusion of moving particles. Hence, another significant dispersion curve, Dκ^2 versus wave vector, κ, has been plotted in Figure 5(b) with a solid-square curve (-■-). The figure exhibits the variation in the diffusive frequencies that emerged from the κ–dependent form of the diffusion coefficient, which has turned out to be an adjustable realistic parameter in the present form of theory. As is evident from the figure, when compared to

time through the diffusion of moving particles. Hence, another significant dispersion curve, Dκ^2 versus wave vector, κ, has been plotted in Figure 5(b) with a solid-square curve (-■-).

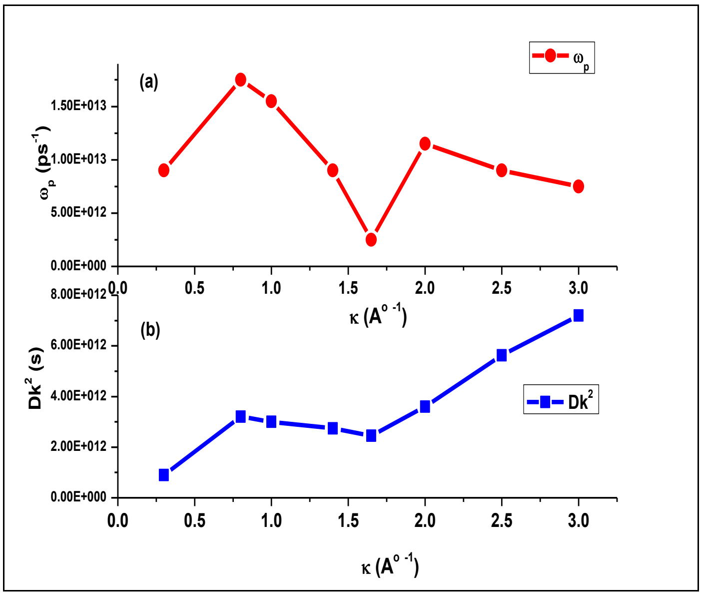

Figure 5(a): ω_p versus k , for liquid Rb at 338 K: (—●—) deduced from the current correlation functions from present theory.
Figure 5(b): Variation of Dκ^2 with κ : (—■—), present theory.

The figure exhibits the variation in the diffusive frequencies that emerged from the κ–dependent form of the diffusion coefficient, which has turned out to be an adjustable realistic parameter in the present form of theory. As is evident from the figure, when compared to the other dispersion curve of fig 5(a), the two are in a synchronized pattern, except that the later curve is devoid of the secondary peak and rather keeps on increasing with increase in wave vector, for κ > 1.65 Å^{-1}. Further, the diffusive frequencies are lower on scale when compared to the collective mode frequencies.

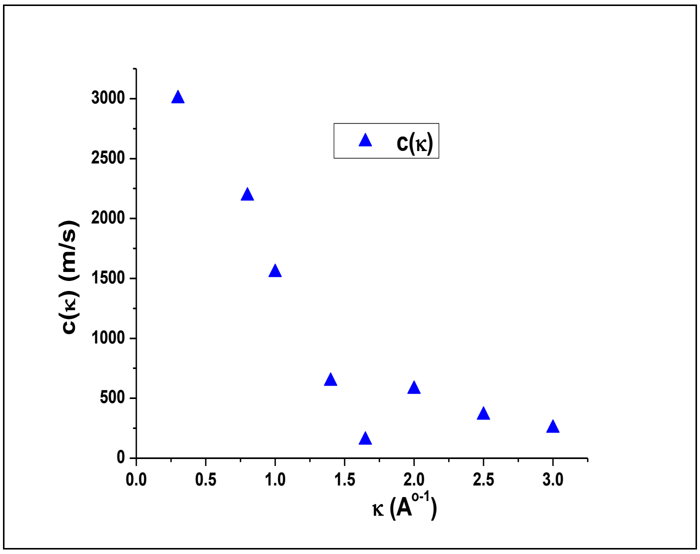

Figure 6: Velocity of sound in liquid potassium at 338 K versus, wave-vector, κ : (▲) (as depicted from figure 5(a)).

Figure 6 presents the variation of κ–dependant form of the velocity of sound, c(κ), has been shown by solid triangles (▲), obtained from ω_p versus κ, the dispersion relation of figure 5(a). For $\kappa \rightarrow 0$, in the linear region of the dispersion curve, value for velocity of sound turns out to be 1771 m/s, and turns to be aligned with experimental measurements [27], reported to be nearly 1790 m/s.

6. Conclusion and Future Scope

This can be concluded from the theoretical investigation that the modified microscopic theory is able to predict the dynamical structure factors and the complete dynamics of a strongly correlated fluid of potassium at 338 K. The theory in the modified form offers an extensive improvement over the earlier microscopic theory. This approach takes into account the particle correlations by defining a relaxation time through the diffusive motion of interacting particles, which enables the evaluation of significant dynamical properties, including collective modes, the diffusion coefficient, and the sound velocity.

Data Availability

The data generated is included in the manuscript.

Conflict of Interest

The author declares no competing interests.

Funding Source

None

Authors' Contributions

Grima Dhingra: conceptualization, calculations, manuscript writing with figures preparation, reviewing and editing

Acknowledgements

None

References

[1] Landau and Plaezek "Structure of the undisplaced scattering line", *Phys. Z. Sowj. Un.*, Vol.**5**, pp.**172**, **1934**.

[2] I.M. de Schepper and E.G.D. Cohen, "Collective modes in fluids and neutron scattering", *Phys. Rev. A* , Vol.**22**, pp.**287-289**, **1980**. ttps://doi.org/10.1103/PhysRevA.22.28

[3] A. Rahman, "Correlations in the Motion of Atoms in Liquid Argon", *Phys. Rev. A,* Vol.**136**, pp.**405-411**, **1964**. https://doi.org/10.1103/PhysRev.136.A405

[4] J. P. Hansen and I. R. McDonald, *Theory of simple liquid,* Academic, London **1986**. ISBN-13: 978-0123870322

[5] M. Sayem, R. D. Murphy, "*Temperature Dependence of Transport Properties of Liquid Sodium and Potassium*", Phy. Chem. Liq., Vol.**40**, No.**4**, pp.**469-475**, **2002**.

[6] C. Chen, H. Eyring, "*Significant Liquid-Structure Theory of Viscosity and Self-Diffusion of the Alkali Metals*", Proc. Nat. Acad. Sci., USA, Vol.**69**, pp.**1342-1345**, **1972**.

[7] J.R.D. Copely and J.M. Rowe, "Short-Wavelength Collective Excitations in Liquid Rubidium Observed by Coherent Neutron Scattering", *Phys. Rev. Letters*, Vol.**32**, pp.**49-52**, **1973**. https://doi.org/10.1103/PhysRevLett.32.49

[8] C. Morkel and W. Glaser, "Single Particle Motion in Liquid Sodium", *Phys Rev. A,* Vol.**33**, pp.**3383-3389**, **1986**. https://doi.org/10.1103/PhysRevA.33.3383

[9] E. Burkel, *Inelastic Scattering of x-rays with very high energy resolution*, Springer-Verlag, Berlin, **1991**. ISBN-13: 978-3662150092

[10] M. Monaco,T. Scopigno, G. Monaco et al., "*Collective Dynamics in Molten Potassium: An Inelastic Scattering Study*", Journal of chemical physics, Vol.**120**, No.**17**, pp.**8089-8094**, **2004.**

[11] J. Hubbard and J.L. Beeby, "Collective motion in liquids", *J. Phys. C,* Vol.**2**, pp.**556-574**, **1969**. https://doi.org/10.1088/0022-3719/2/3/318

[12] S.P. Tewari and Surya P. Tewari, "Theory of collective motion in liquids", *J. Phys. C: Solid State Physics*, Vol.**8**, pp.**L569-L572**, **1975**. https://doi.org/10.1088/0022-3719/8/24/001

[13] S.P. Tewari and Surya P. Tewari, "Theory of collective motion in liquids", *J. Phys. C: Solid State Physics*, Vol.**8**, pp.**L569-L572**, **1975**. https://doi.org/10.1088/0022-3719/8/24/001

[14] S.P. Tewari, J. Sood and P. Tandon, "Collective dynamics of liquid alkali metals Cs and Rb", *J. Non-Crystalline Solids*, Vol.**281**, pp.**72-80**, **2001**. https://doi.org/10.1016/S0022-3093(00)00437-3

[15] S.P. Tewari and Surya P. Tewari, "Theory of long wavelength collective motion in liquids", *Phys. Letters*, Vol.**65A**, pp.**241-243**, **1978**. https://doi.org/10.1016/0375-9601(78)90162-7

[16] S.P. Tewari, G. Dhingra and P. Silotia, "Collective Dynamics of a Nanofluid: Fullerene, C_{60}", *International J. of Mod. Phys. B.*, Vol.**24**, pp.**4281-4292**, **2010**. https://doi.org/10.1142/S0217979210055974

[17] S.P. Tewari, and J. Sood, "Collective Dynamics of Liquid Al", *Modern Phys. Letters,* Vol.**18**, pp.**811-816**, **2004**. https://doi.org/10.1142/S0217984904007293

[18] G. Dhingra, "Dynamical Modes in Liquid Mercury along Liquid-Vapour Curve", *International Journal of Scientific Researchin Multidisciplinary Studies*, Vol.**8**, Issue.**9**, pp.**01-05**, **2022**. https://doi.org/10.26438/ijsrpas/v8i9.15

[19] S.P. Tewari and Surya P. Tewari, "Zero frequency dynamical structure factor of liquids", *Phys. Letters*, Vol. 56A, pp.**99-100**, **1976**. https://doi.org/10.1016/0375-9601(76)90157-2

[20] G. Dhingra, "Microscopic Transport Phenomena in a Liquid Alkali Metal: K^{39}", *International Journal in Scientific Research in Physics and Applied Sciences*, Vol.**7**, Issue.**1**, pp.**56-59**, **2019**. https://doi.org/10.26438/ijsrpas/v7i1.5659

[21] S.P. Tewari, G. Dhingra, P. Silotia and J. Sood, "Theory of collective dynamics of liquid polyvalent metal: Hg", *Phys. Letters A,* Vol.**368**, pp.**412-418**, **2007**. https://doi.org/10.1016/j.physleta.2007.04.035

[22] G. Dhingra, "Correlated Motion of Particles in Liquid Sodium Metal", *International Journal of Scientific Research and Reviews*, Vol.**8**, Issue.**1**, pp.**1085-1091**, **2019**.

[23] S.P. Tewari, G. Dhingra, P. Silotia and J. Sood, "Microdynamics of a monoatomic liquid metal", *J. Non-Crystalline Solids* Vol.**355**, pp. **2522-2527**, **2009**. https://doi.org/10.1016/j.jnoncrysol.2009.08.014

[24] J.M.G. Mirannda, "A molecular dynamics Study of liquid potassium at 340 K", *J. Phys. F: Met. Phys.*, Vol.**16**, pp.**1-10**, **1986**. https://doi.org/10.1088/0305-4608/16/1/007

[25] A.J. Greenfeld, J. Wellendorf and N. Wisser, "X-Ray Determination of the Static Structure Factor of Liquid Na and K*",* *Phys. Rev. A,* Vol.**4**, pp.**1607-16**, **1971**. https://doi.org/10.1103/PhysRevA.4.1607

[26] J.L. Bretonnet, N. Jakse, "Use of integral-equation theory in determining the structure and thermodynamics of liquid alkali metals", *Phys. Rev. B,* Vol.**50**, pp.**2880**, **1994**. https://doi.org/10.1103/PhysRevB.50.2880

[27] M.J. Hujiben and W. van der Lugt, "X-ray and Neutron Diffraction from Liquid Alkali Metals", *Acta Cryst. A*, Vol.**35**, pp.**431-445**, **1979**. https://doi.org/10.1107/S0567739479001042

[28] A. D. Pasternak, "Sound-wave velocities in liquid alkali metals studied at temperatures up to 150^0c and pressures up to 0.7 Gpa", *Mater. Sci. Eng.* **3**, pp.**65**, **1969**. https://doi.org/10.1016/0025-5416(68)90019-0

AUTHORS PROFILE

Dr. Grima Dhingra is an alumni of Department of Physics and Astrophysics, University of Delhi. She completed her M.Sc. in 2002 and her Ph.D. in 2009 from the department of Physics and Astrophysics, University of Delhi. She gained her doctorate degree with specialization in Condensed Matter Physics. Her core thrust areas of research include Fluid Dynamics, Molecular Dynamics Simulation, Cryptography and Plasma Physics. The peer has over fifteen research papers published in peer-reviewed and indexed international journals. She has presented many of her research papers in different international and national conferences. Dr. Grima has conducted successfully minor project during 2012-14 granted by UGC to her as principal investigator. She is a life member of Indian Crystallographic Society (ICS) and also of Materials research society of India (MRSI). She is working as Associate Professor in the Department of Physics, M.D. University, Rohtak, Haryana and bears an experience of 3 years of UG and 14 years of PG teaching along with a research experience of 17 years.