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Research Article

Dynamical Structure Factors of an Alkali Metal: Liquid Rubidium

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Abstract— Theoretical calculations for the coherent dynamical structure factors of an alkali metal, liquid rubidium (^{85}Rb) at a temperature of 338 K, fairly above the melting temperature of liquid metal and corresponds to a mass density of **1.45 g/cm³**. Are reported. Melting temperature of rubidium is 312.45K, and at the considered temperature of 338 K, the liquid system is 0.945 times rarer as compared to that at room temperature. Theoretical results are provided for a wave-vector range of 0.2 $Å^{-1}$ to 5.0 $Å^{-1}$. The wave-vector range corresponds up to the primary and secondary maxima positions in the structure factor of liquid at the considered physical conditions of temperature and density. The modified microscopic theory of collective dynamics in simple liquids is applied for the present computations. The theory turns out to be a self-consistent approach and produces the equilibrium dynamics of a liquid with the acquaintance of the inter-particle interaction. Along with the dynamical structure factor, other dynamical properties; diffusion coefficient the dispersion relation and sound velocity liquid rubidium under these conditions, have also been reported.

Keywords— Dynamical structure factor, Alkali metal, Inter-particle interaction potential, Diffusion coefficient; Modified microscopic theory

1. Introduction

The equilibrium dynamics of fluids, unlike crystalline ordered state of solids and complete disorder of ideal gases, is intensively complex and is much harder to explore. These intricate dynamical states of any fluid, characterized by the simultaneous presence of single as well as collective motion can be expressed through space-time dependent correlation function. The dynamical structure factor is the Fourier transform of this Van-Hove space-time dependent correlation function [1]. The dynamical structure factor describes the response of any liquid to a weak disturbance and therefore provides a detailed vision of the collective behaviour of its constituent atoms.

Experimental methods like inelastic X-ray scattering (IXS) and thermal neutron inelastic scattering (INS) are frequently used to examine the collective motion of interacting particles. However, these techniques have certain limitations. In INS, the substantial incoherent scattering due to neutron-nucleus interactions confounds the coherent and incoherent dynamical structure components. In contrast, IXS [2] can provide purely coherent data when performed with high-resolution synchrotron radiation sources. Liquid rubidium (Rb), with an atomic mass of 85.47 a.m.u., is a far superior coherent scatterer [3] of neutrons as compare to liquid sodium [4] and liquid cesium [5], the other two alkali metals, boasting a coherent to incoherent scattering cross-section ratio of around 1800 (values for cesium and sodium are 16.0 and 0.99, respectively) and the INS spectra of liquid Rb is predominantly coherent. This makes rubidium an excellent candidate for the prediction of the collective modes in a strongly correlated liquids. Some of the experimental studies from neutron scattering are available in the literature [6-8] wherein liquid rubidium displays a well-known three-peak structure in its dynamical structure factor, even at high momentum transfers, similar to the behaviour observed in the hydrodynamic regime. However, these studies essentially are confined to the closest vicinity of the melting temperature only and higher temperature dynamical states of the liquid alkali remained unreported. To the best of my knowledge, no experimental data for collective dynamics at this temperature and density conditions of Rb in its liquid state have been provided by any of the INS or IXS studies.

This paper is described in five sections. Section 1, provides an introductory definition of the research work carried in the present study and section 2 reviews the earlier work done in the field. In section 3, mathematical formalism for the applied theory is described. Section 4, carries all the results from present computations, Figures and the associated discussions for the outcomes. In section 5, conclusions drawn from the study and the future scope are narrated.

2. Related Work

The current predictions are based on the modified microscopic theory, where the microscopic behaviour of any condensed system is examined to determine the density response function. This complex function, which includes both real and imaginary parts, describes the space-time-dependent fluctuations in the fluid's density in response to a weak perturbation. Through a Fourier transform, the imaginary part of the density response function and the dynamical structure factor are connected via the Fluctuation-Dissipation theorem, which is the prime concern of this study. To include inter-particle correlations that were not addressed in the previous theory, a characteristic relaxation time is introduced [9]. This time is dependent on several physical factors, including the static structure factor, density, temperature, mass, interaction potential. In this theory, the diffusion coefficient is made to be a wave vector dependent entity which acquires a specific value for each wave-vector. Hence, while incorporating appropriate representation of the intermediate self-scattering function, the number of arbitrary parameters are reduced through such an adjustment.

The modified model has been successfully applied to describe the collective dynamics of several liquids [10-19]. The present communication represents the prediction of the collective dynamics of liquid rubidium at a temperature of 338 K, aiming to describe the response of the liquid to an external radiation and compute the dynamical structure factor for liquid Rb.

3. Theory and Mathematical Formalism

Microscopic theory analyzes the density fluctuations to describe the motion of particles. To gain a deeper understanding of the complex space-time-dependent correlation functions, they are defined and approximated to obtain results for the dynamical structure factor. In this earlier version of the theory distinct time correlations were not considered while calculating the dynamical structure factors. As a result, the dynamical structure factors produced were excessively damped and did not match the experimentally observed spectral line shapes. To address this limitation, Tewari et al. [9] attempted to modify the theory by entailing a characteristic relaxation time which takes in to account for the missing correlations. The microscopic theory, in its modified version, has successfully explained the dynamical structure factors of several liquids.

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:

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

Where, $\beta' = D\,\kappa^2$, 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:

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

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:

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

Here, $V(r)$ 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 described in the above section of mathematical formalism, evolution of any fluid towards the equilibrium dynamics can be computed using the modified microscopic theory which further requires the necessary information about the inter-particle interaction potential with which the constituent particles are interacting with each other. One, therefore, has to find out a suitable interaction potential, of considered liquid at given physical conditions. In order to work out the dynamical structure factors this is more appropriate to entail an interaction potential which is generated through or is connected to the static structure factor instead of other methods including algebraic mathematical work out. For this reason, an interaction potential acting between constituent particles of liquid rubidium as proposed by Bretonnet and Jakse [20] at a nearby temperature (m.pt. 312 K) has been key in to present calculations. However, few other attempts to generate inter-particle interaction potential of liquid Rb, are also [21] available from the literature, this form of the potential has reproduced experimentally, measured static pair correlation function g(r), Fourier transform of the static structure factor [8] of liquid rubidium and hence, has emerged as an optimal selection for the present work. The suggested interaction potential is comprised of hard core and long range oscillator parts, acquires a typical form for liquid alkali metal. The interaction potential for liquid Rb has been compared to the inter-particle interaction potential of liquid lithium (Li) [22], which is the lightest among the alkali metals and are shown in Figure 1: solid curve (———) liquid Rb at 319 K and dash-dot curve (– · –) NPA potential for liquid Li at 475 K. The interaction potentials compared in Figure 1 are near their melting temperatures and can be observed to be different from each other. The depth for interaction potential, corresponding to the minimum of the curve, of liquid rubidium is much shallower than that for liquid Li, whereas oscillations occurred due to the presence screening effect of degenerate gas of electrons, exhibit wider variations in liquid Rb as compared to that in lithium. This difference can be attributed to the difference in their atomic sizes and to the difference in r_s, (r_s for Li = 1.73Å and Rb =5.043 Å). The larger atomic radius of a Rb atom has also been resulted in a larger hard core as compared to the Li, which has the smallest atomic radius among alkali metals.

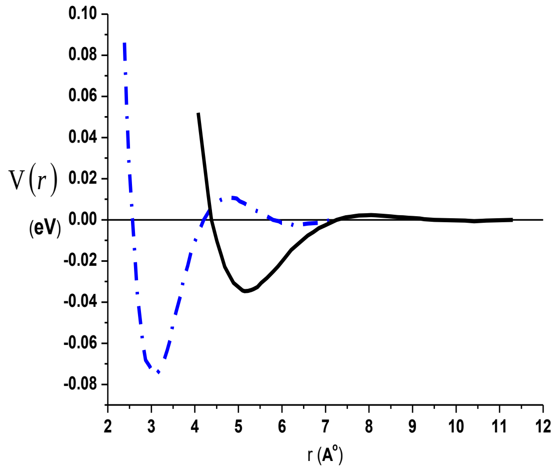

Figure 1: Variation of $V(r)$ with inter-atomic distance *r*: **(———)** liquid rubidium at 319 K; (— —) liquid Li at 475 K.

This form of inter-particle interaction potential, yields the maximum Einstein frequency ω_E , through mathematical equation (5),and r_o, from expression (6), for liquid Rb, respectively as: 8.52×10^{12} s^{-1} and 4.66 Å. The pair distribution function g(r), used in these calculations is that obtained from the experimental data of static structure factor [22] when Fourier transformed and also regenerated through this form of the interaction potential of liquid Rb [20]. ω_E , r_o and ω_κ as calculated from the expression (4), are substituted into the mathematical equation (2) to calculate the relaxation time. This form of single characteristic relaxation time, τ(κ) is built-in to the modified microscopic theory to take in to account the distinct particle correlations at different κ values. τ(κ) essentially considers the wave-vector-dependent correlations to describe the time-evolution of distinct properties such as particle positions or densities. Essentially, the time scale for the system to regain equilibrium after a perturbation is represented.

The diffusion coefficient, D, is appeared as a parameter to certify the justification of the zeroth sum rule and is governed by expression (2). The zeroth sum rule is typically a normalization condition that ensures the correct shapes of the dynamical structure factors over all ω–ranges. Hence, the suggested modification in the microscopic theory leads to fulfillment of all sum rules of liquids. the detailed dynamical structure factors S(κ,ω) is now calculated using the relaxation time and diffusion coefficient, These structure factors are defined to describe the fluctuations of the system in both space and time, and they are crucial for understanding the dynamic behaviour of a system. They are derived using expression (1), which likely relates S(κ,ω), τ(κ), and diffusion coefficient, *D*.

Through expression (1), the dynamical structure factors for wave-vector values, ranging from 0.2 Å^{-1} to 5.0 Å^{-1}, have now been computed. And the results to demonstrate their variation with frequency ω, have been plotted in Figure 1 for κ=0.2 Å^{-1}; κ= 0.6 Å^{-1}; κ= 1.0 Å^{-1} and κ= 1.75 Å^{-1} with a solid-square curve (− ■ −) and in Figure 2 for κ= 2.5 Å^{-1}; κ= 3.0 Å^{-1}; κ= 4.0 Å^{-1} and κ= 5.0 Å^{-1} with a solid-square curve (− ■ −). In this process, effective diffusion coefficient, D_{eff} remains constant and is equal to the diffusion coefficient given in expression (2), without any variation with frequency. As shown in two figures, increase in wave-vectors has lead to damping of the dynamical structure factors are damped and display features only central peaks, without shoulder peaks, except at κ= 0.2 Å^{-1}. For κ> 0.6 Å^{-1}, Brillouin peaks have not appeared. As no experimental data at considered temperature of 338 K is available, the evaluated data is compared with the data from the INS study [3] at melting point, 312 K. These results from previous experimental study have been shown in Figure 1: with solid circles (●) at κ= 0.63 Å^{-1} and κ= 1.01 Å^{-1}. The comparison indicates the damping of structures with an increase in the temperature as near melting point, the dynamical structures are rather sharp and exhibit shoulder peaks up to κ=1.01 Å^{-1}.

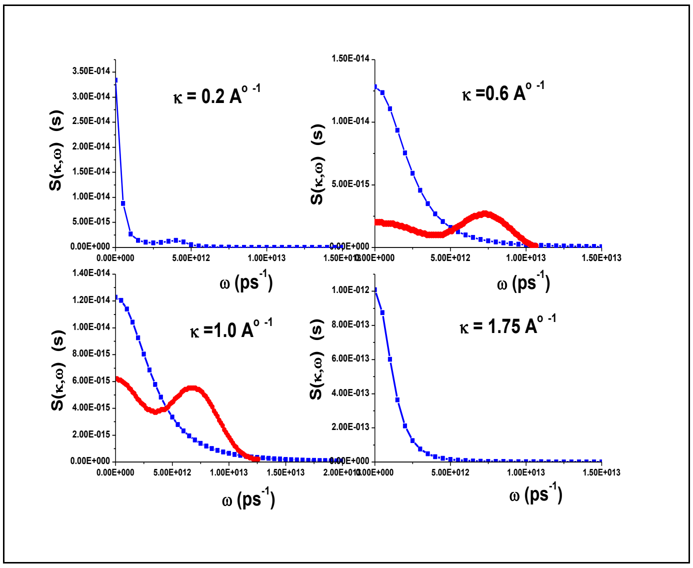

Figure 2: Dynamical structure factor, $S(\kappa,\omega)$ versus frequency, ω, for liquid rubidium at 338 K: (—■—) present theory at κ=0.2 Å^{-1}, κ= 0.6 Å^{-1}, κ= 1.0 Å^{-1} and κ=1.75 Å^{-1}; (●) experimental results [6] at 319 K.

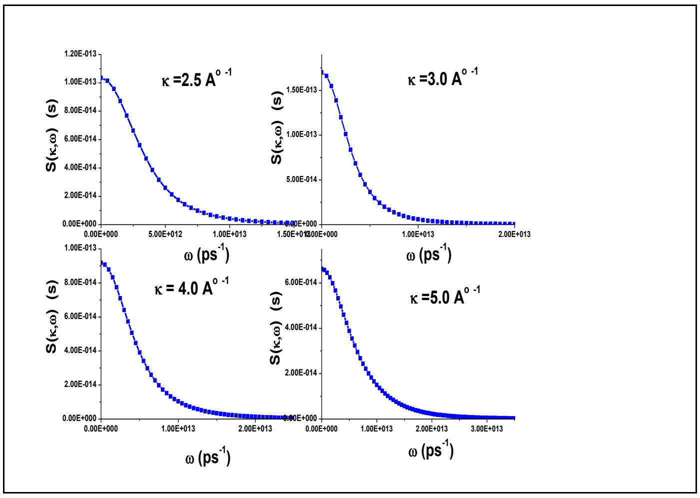

Figure 3: Dynamical structure factor, $S(\kappa,\omega)$ of liquid rubidium at 338 K versus frequency, ω: (—■—) present theory at κ=2.5 Å^{-1}, κ= 3.0 Å^{-1}, κ= 4.0 Å^{-1} and κ=5.0 Å^{-1}.

The only fitting parameter in the theory, the self-diffusion coefficient, acquires wave-vector dependant form, have been obtained in the process of generating dynamical structure factors. The vital sum rule followed by the generated structures, the, zeroth sum rule was not justified in that generated by the older microscopic theory [23]. Further, the coefficient of diffusion is essentially connected to the estimation of the relaxation time. In Figure 4(a), the variation in $[D\kappa^2]^{-1}$, representing the diffusive time occurred in the present theory, has been drawn as against the wave-vector, κ: solid curve (———). In Figure 4(b), the relaxation time, as described and calculated from the expression (2), has been plotted against wave-vector, κ: with solid curve (———).

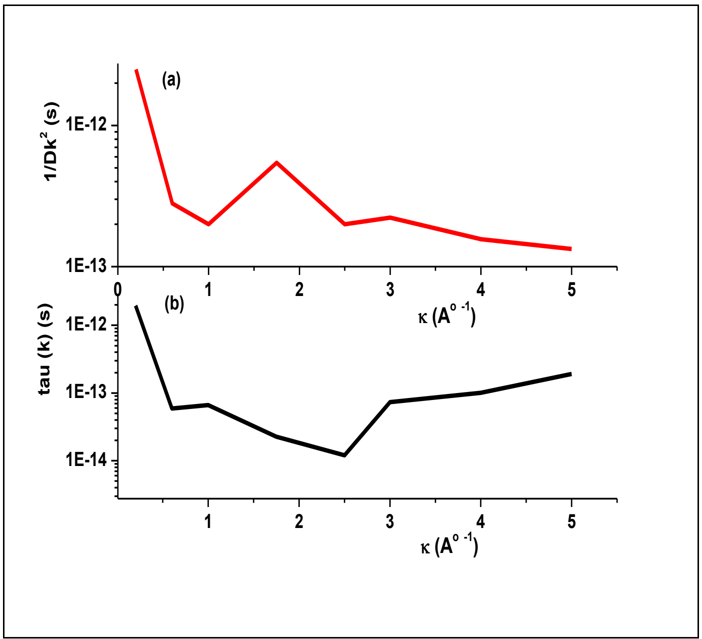

Figure 4(a): Variation of **1**/Dκ^2 with κ : (———).
Figure 4(b): Variation of characteristic relaxation time with κ: (———).

This can be seen from the figure that for κ< 1.0 Å^{-1} the diffusive time decreases by an order and thereafter, for κ= 1.0 Å^{-1} to 5,0 Å^{-1}, remains varying in half an order only. The characteristic relaxation time, on the other hand, decreases to an order with an increase in κ up to κ~0.5 Å^{-1}., then to another an order up to κ =2.5 Å^{-1}, and increases within half an order thereafter for higher wave vectors. The overall variation in $[D\kappa^2]^{-1}$ is about an order, whereas relaxation time varies for two orders in the entire κ–range. This can further be observed that the relaxation time for entire κ-range, specifically for 0.6 $Å^{-1} \leq \kappa \leq 3.0$ $Å^{-1}$, diffusive time leads by more than half an order to the relaxation time.

In Figure 5(a), the variation of ω_p, the collective mode frequencies, with κ under different considerations, have been plotted: solid squares (■) ω_p from present theory; and solid curve (――――) ω_κ from expression (4). The values of ω_p have been deduced from the current-2 correlation functions, which are related to the evaluated dynamical structure factors from expression (7). The frequencies of collective modes correspond to the peak positions of the current-2 correlation function for a given wave-vector. As seen in the figure, the collective mode frequencies initially increase with an increase in the wave-vector, to a maximum at nearly $\kappa = 1.0$ $Å^{-1}$, followed by a decrease up to $\kappa = 2.5$ $Å^{-1}$ to attain a minimum here, and with further increase in the wave-vector increases thereafter. This pattern reflects the typical trend for the variation of the dispersion relation. The variation of wave-vector dependant frequencies ω_κ with κ is similar in pattern to the former frequency except that of exhibiting a second minimum at nearly $\kappa = 3.0$ $Å^{-1}$. Moreover, they are larger as compared to the other frequencies, ω_p.

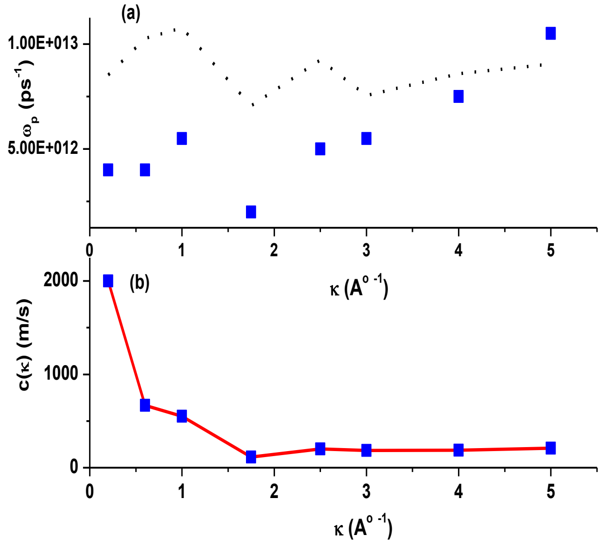

Figure 5(a): Dispersion relations for liquid Rb at 338 K under various considerations: (■) ω_p deduced from current correlation function; (- - -) ω_κ. from expression (4).

Figure 5(b): Velocity of sound in liquid rubidium at 338 K as depicted from figure 5(a) vs. wave-vector, κ: (―■―).

The sound velocities as calculated from the dispersion relation ω_p versus κ (shown in Figure 5(a)) have been displayed in Figure 5(b) represented by a solid-square curve (-■-). The results have been plotted against wave-vector, κ. Theoretically, one may expect these computed sound velocities to be aligned with the experimentally measured values in the region where κ approaches 0. The sound velocity depicted from the linear region of the dispersion curve, corresponding to κ near 0, turns out to be 1190 m/s as against the experimental results (~1247 m/s) [24].

5. Conclusion and Future Scope

This can be concluded from the study that the modified microscopic theory is able to provide the collective dynamics of liquid Rb at 338 K and offers a substantial enhancement over the older theory. This theory includes the inter-particle interactions and inculcates the correlations between distinct particles by defining a characteristic relaxation time that incorporates inter-particle interactions. It enables the determination of other important properties including the diffusion coefficient, collective modes, and sound velocity.

The theory can be applied further for the prediction of collective dynamics of a variety of other fluids subject to different physical conditions.

The reported results can further be worked out to calculate other transport properties of the liquid potassium.

Data Availability

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

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None

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