

## Dynamical Structure factor by using Memory Function Approach

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**ABSTRACT:** In the present study the dynamical structure factor of liquid sodium at 390 K i.e. slightly above melting point has been studied by using a memory function having single relaxation time, whose functional form depends on the wave number and thermodynamic state of the system. The parameters of memory function are related to the sum rules of the dynamical structure factor up to sixth order. It has been found that the dynamical structure factor of liquid Na is well explained with new model of memory function over a wide range of wave vector, 1.5-14.6 nm<sup>-1</sup>.

**Key Words:** Dynamical Structure factor, memory function, relaxation time, sum rules, wave number

### INTRODUCTION

The collective modes in liquids can be studied through their dynamical structure factor,  $S(q, \omega)$  which contains complete information about the dynamics of the liquids and can be obtained experimentally from neutron or inelastic X-ray scattering (IXS) experiments. Recently inelastic X-ray scattering experiments have been performed<sup>1</sup> for liquid Al, Li, Na and Ga etc. for the purpose of studying the collective excitations at wave vectors below the first sharp diffraction peak. Theoretically, memory function (MF) formalism is one of the methods to describe the collective dynamics, as dynamical structure factor can be linked to the density-density time correlation function. A significant role has been played by Mori's memory function formalism<sup>2</sup> in the study of dense fluids. The Mori's formalism reduces the problem of calculation of time correlation function to the calculation of MF. Many forms of MFs like Gaussian, simple exponential, hyperbolic secant and square of hyperbolic secant have been used to predict transport coefficients of classical fluids. These suggested forms were unable to predict transport coefficients with uniform accuracy over complete range of temperature and density. It has been argued that two or three time scale decay of memory function is needed to understand the collective phenomenon in liquid metals.

However, on the other hand a semi empirical model which is based on the extension of hydrodynamic model to the viscoelastic region satisfying the first four non vanishing sum-rules has been able to explain successfully<sup>3</sup> the line spectra for liquid metals Li, Na and Al. Also recently, we have derived a memory function with single relaxation time whose functional form depends on the wave number and thermodynamic state of the system. This MF not only satisfies the first four sum-rules but also predicts the next higher order sum rule with reasonable good agreement with known values. In the present work we use this new form of the MF with single relaxation time to study the collective excitations in liquid Na at 390 K. The parameters of the memory function can be related to the sum rules of the dynamical structure factor up to eighth order. It is observed that even single relaxation time model for the memory function can do fairly well to explain the experimental X-ray scattering data for the liquid alkali metals in the small wave vector region below the first sharp diffraction peak, where the quantum correction from the detailed balance factor is also taken into account, provided two of the parameters of the MF are fitted.

### THEORETICAL FORMALISM

The collective dynamics of a liquid can be studied through density correlation function,  $F(q, t)$  defined as

$$F(q, t) = (1/N) \sum_{i,j} \langle e^{-iq(r_i(0) - r_j(t))} \rangle \quad (1)$$

where  $N$  is the total number of particles each of mass  $m$ ,  $r_j(t)$  denotes the position of the  $j$ th particle at time  $t$ . The dynamical structure factor,  $S(q, \omega)$  is the frequency spectrum of  $F(q, t)$ . Structural features are accounted for by the initial values  $F(q, t=0) = S(q)$ , known as static structure factor which come from experiments. The quantity  $F(q, t)$  satisfies an integro-differential equation of the form

$$\ddot{F}(q, t) + \omega_0^2(q)F(q, t) + \int_0^t M_2(q, t - \tau) \dot{F}(q, t - \tau) d\tau = 0 \quad (2)$$

where  $\omega_0^2 = q^2 k_B T / m S(q)$ , is the second frequency moment of  $S(q, \omega)$  and the kernel  $M_2(q, t)$  is the correlation function of random forces and is known as the MF associated with  $F(q, t)$ . The dynamical structure factor can be related to the fourier transform of  $F(q, t)$  as

$$S(q, \omega) = \frac{1}{\pi} \text{Re} \int_0^\infty \exp(-i\omega t) F(q, t) dt, \tag{3}$$

using above equations,  $S(q, \omega)$  can be written in terms of real,  $M_2'$  and imaginary,  $M_2''$  parts of the MF as

$$S(q, \omega) = \frac{S(q)}{\pi} \frac{\omega_0^2 \tilde{M}_2''(q, \omega)}{A^2 + (\omega \tilde{M}_2'(q, \omega))^2} \tag{4}$$

where  $A = (\omega^2 - \omega_0^2(q) + \omega \tilde{M}_2'(q, \omega))$ .

In order to calculate  $S(q, \omega)$  from Eqn. (4),  $M_2(q, t)$  is required. The  $M_2(q, t)$  satisfies an equation similar to that of Eqn. (2), but involving higher order MF. By employing suitable approximation, we have derived<sup>4</sup> a form of MF given as

$$M_2(t) = \delta_2 \text{sech}^\nu \left( \sqrt{\frac{\delta_3}{\nu}} t \right), \tag{5}$$

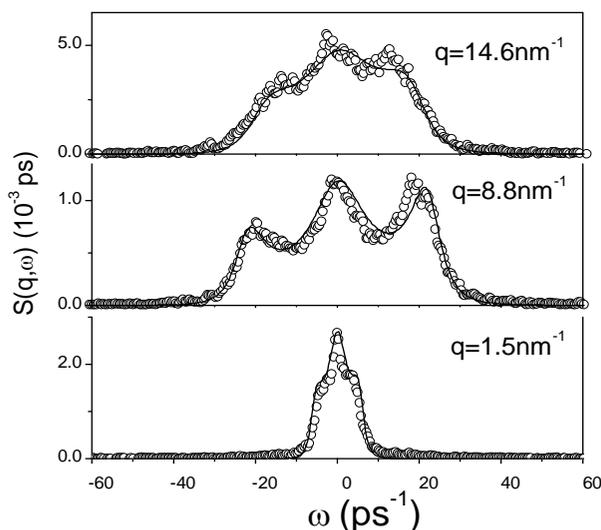
with  $\nu = \frac{2\delta_3}{\delta_4 - 2\delta_3}$ , where  $\delta_2$ ,  $\delta_3$  and  $\delta_4$  are related to frequency moments of  $S(q, \omega)$  upto eighth order. Taking the Fourier -Laplace transform of the above equation and calculating the real and imaginary parts of memory function and using in Eqn. (4) we get  $S(q, \omega)$ . It is worth noting that for comparing our results with experimental results, we have used following approximation, which connects the experimental  $S_Q(q, \omega)$  with its classical counter part calculated from equation (4) as

$$S_Q(q, \omega) = S(q, \omega) \frac{\beta \hbar \omega}{1 - \exp(-\beta \hbar \omega)}$$

where  $\beta = 1/k_B T$  and  $\hbar$  is planck's constant.

**RESULTS AND DISCUSSION**

In order to calculate  $S(q, \omega)$ , we require  $S(q)$ ,  $\delta_2$ ,  $\delta_3$  and  $\nu$  as inputs. For  $S(q)$ , we have used experimental values<sup>1</sup> and for  $\delta_2$  we have used values within error bar evaluated in approximate fashion<sup>5</sup>. To calculate  $\delta_3$  and  $\nu$ , which are related to sixth and eighth order sum rules of  $S(q, \omega)$ , we require not only interatomic potential, but also static correlation function up to fourth order. Since, the aim of the present work is to investigate whether a MF with more number of parameters can explain  $S(q, \omega)$ . The values of  $\delta_3$  and  $\nu$  are fitted. The results of  $S(q, \omega)$  obtained for Na at 390 K are compared with IXS data for  $q=1.5, 8.8$  and  $14.6 \text{ nm}^{-1}$  in Fig. 1. It can be seen from the figure that a good agreement with IXS data has been achieved over a wide range of wave-vector.



**Fig.1** IXS data of liquid Na at 390 K is represented by open circles and solid line represents the results of our model.

It is important to note here that the MF given by Eqn. (5) is involving additional parameter  $\nu$ , which is wave number dependent. The value of different values of  $\nu$  obtained in fitting procedure suggests that the MF may have different forms at different wave numbers.

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