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Study of structure factor of interacting bosons with reference to properties of liquid He^4 below Lambda Transition Temperature

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ABSTRACT

The structure factor for the interacting Bose system at finite temperatures below the Lambda-transition temperature of liquid He^4 has been studied for two types of interacting potentials using a theoretical formulation due to Isihara [Physica B (Netherlands), 106 (1981) 161] and Isihara and Samulski [Physica A (Netherlands), 86 (1977) 257]. In our work we have considered liquid He^4 below its Lambda transition temperature which makes it imperative for us to consider the important aspects of much body interaction by taking recourse to the reaction matrix formalism of many body theories. We expect that our work will provide some additional inputs to the theoretical studies made till date for derivation of the energy excitation spectrum and structure factor for a system of interacting Bore Assembly.

INTRODUCTION

The study of the structure of liquid involves a quantity called structure factor which can be defined as a measure of the diffraction produced by the sample under study, compared to the diffraction that would be produced by an ideal gas. He^4 liquefies from gas to liquid at 5.2K above absolute zero temperature at normal pressure. The super fluid phase transition happens at 2.2K. The density temperature function has a slop discontinuity there; this means a discontinuous thermal expansion coefficient. There is also a sudden change in the dielectric constant. The specific heat at constant volume has a singularity at 2.19K that looks like the Greek letter Lambda. Hence the name "Lambda point". Liquid He^4 called "He-II" below the Lambda point creeps along thin films and flows through narrow tubes with zero viscosity below a critical speed. Fritz London [1] noted the possible connection to the Bose-Einstein condensation of an ideal gas which predicts a Lambda point at 3.13K. Landau [2] in 1941 made a theory good near absolute zero, but not near the Lambda point. Feynman's first super fluid paper argued that in spite of the inter-atomic interactions, super fluid helium was a Bose-Einstein condensate similar to what happens in the ideal gas where the interactions are absent. Feynman's [3] second super fluid paper in 1953 looked at the ground state many atom wave function that dominates the behavior of the liquid near absolute zero. The problem is to construct an excited state. He argued, like Landau in 1941, that the lowest energy excitations were compression sound waves whose quanta are longitudinal phonons with no energy gap. Additional particle-like must have an energy gap and an effective mass. Feynman's [3] third super fluid helium paper appeared in 1954 on the excited may-atom wave-functions.

He^4, in its liquid phase, has another phase transition called Lambda transition which divides the liquid into two distinct phases. , He-I and He-II. Kamerlingh Onnes [5], shortly after he liquefied helium in 1908 noted that the density of the liquid appeared to pass through an abrupt maximum at about 2.2K decreasing slightly thereafter.

Further investigations revealed that the critical temperature is 2.176K and that it represents a transition to new state of matter known as He-II, in which, the heat conductivity is very large of the order of $3x10^6$ times greater and the viscosity enormously less than that at a higher temperature. The state has no latent heat and its specific heat curve is discontinuous. The temperature of 2.176K is called the "Lambda Transition Temperature", or briefly as the λ-point. The λ-point gets its name from the λ-like shape of the specific heat curve at the λ-temperature. The isobaric expansion coefficient, vapour pressure and the specific heat all have singularities at the λ-point. The specific heat of the liquid He^4 at higher densities has been measured above 1.2K by Hercus et al. [6] and by lounsmaa et al. [7].

The first theoretical account of the Lambda transition was given by F. London [1,8] who regarded it as the analogue in a liquid of Bose-Einstein condensation predicted for an ideal Bose gas. The excitation models of liquid He^4 put forward by London on the basis of quasi-particle of elementary thermal excitations are well corporate by experimental evidence. Liquid He^4 below its Lambda transition is found to exhibit the rapid thermodynamic changes around 0.6K and the recent theoretical studies on the interacting bosons with a two body potential composed of a hard core followed by two Gaussians have resulted an energy excitation spectrum similar to that of liquid He^4. The potential i.e. the Gaussian equivalent of the Lennard-Jones potential has recently been used by Khanna et al. [9-13], in their study on interacting bosons and properties of liquid He^4.

The calculations in the present work have enabled us to derive the structure factor for the interacting Bose system at finite temperatures below the Lambda-transition temperature of liquid He^4.

MATERIALS AND METHODS

II. THEORETICAL FORMULATION:

We consider a system of N interacting bosons enclosed in a volume V such that the density ρ is held constant even when N and V approach unity. The bosons are assumed to be interacting via either of the following two forms:

(a) Hard core followed by a combination of both repulsive and attractive Gaussian potentials (which is the Gaussian equivalent of the Lennard-Jones potential) [13] given by

$$U(r) = \begin{cases} +\infty, & r < a \\ 4\varepsilon_0 \left[\exp\left(\frac{r-a}{\mu_R}\right)^2 - exp\left(\frac{r-a}{\mu_A}\right)^2\right], & r \geq a \end{cases} \qquad (1)$$

where a is the diameter of the hard core , ϵ is the depth of the potential and μ_R and μ_A are the repulsive and attractive ranges respectively after the hard core.

(b) Hard core followed by square well is given by

$$U(r) = \begin{cases} +\infty, & r < a \\ -\varepsilon, & a < r < b \\ 0, & r > b \end{cases} \qquad (2)$$

where b is the range of the attractive square well after the hard core.

Now as obtained by Samulski and Isihara [14], the structure factor for a system of bosons interacting via a potential whose Fourier transform is U(q) is given by

(3)

$$S(q) = \frac{\hbar^2 q^2}{2m\varepsilon(q)}\left[1 + 2f\{\varepsilon(q)\}\right]$$

where ε(q) is the excitation energy given by

$$\boxed{\varepsilon(q) = \frac{\hbar C q}{U(0)^{1/2}}\left[U(q) + \frac{\hbar^2 q^2}{4m\rho}\right]} \tag{4}$$

and $$f(\varepsilon) = \frac{1}{e^{\beta\varepsilon} - 1} \tag{5}$$

In equation (4) C is the velocity of sound and $\beta = \frac{1}{kT}$, k being the Boltzmann constant and T is the absolute temperature.

Equation (3) was derived by Samulski and Isihara [14] in their macroscopic theory and it is easily seen that at absolute zero, this equation reduces itself to the well-known Feynmann relation

$$S(q) = \frac{\hbar^2 q^2}{2m\varepsilon(q)} \tag{6}$$

Assuming that in the region q-0, the energy is phonon- like, i.e.

$$\varepsilon(q) = \hbar C q \tag{7}$$

We see that Equation (6) gives

I $$S(q) = \frac{\hbar q}{2mC} \tag{8}$$

sihara [15] in his study on the temperature variation of the structure factor of liquid He^4 adopted a soft potential with a Lennard -Jones type of tail given by

$$U(r) = \begin{cases} V_0, & r < a \\ \varepsilon^*\left\{\left(\frac{a}{r}\right)^{\frac{1}{2}} - \left(\frac{a}{r}\right)^6\right\}, & r \geq a \end{cases} \tag{9}$$

and used the Fourier transform of this potential obtainable from Ref.16. The result obtained is that, for small momentum and in a range of few degrees of temperature, Equation (4) gives

(10)

where

$$\varepsilon(q) = \hbar C q\left[1 + \delta_1 q^2 - \delta_2 q^3 + ...\right]$$

$$\delta_1 = \frac{\hbar^2}{8m^2C^2}\left\{1 - 16\pi a^5 m\rho\hbar^{-2}\left(\frac{V_0}{30} - \frac{\varepsilon^*}{7}\right)\right\} \tag{11}$$

$$\delta_2 = \frac{\pi}{24mC^2}\rho a^6 \varepsilon^* \tag{12}$$

Thus, for smaller q values, the structure factor has been found to be given by

(13)

where $$S(q)/S(0) = 1 + S_1 q^2 + S_2 q^3 \tag{14}$$

$$S_1 = \frac{1}{12}\left(\hbar C / kT\right)^2 - 2\delta_1$$

$$S_2 = 2\delta_2$$

The results obtained for the structure factor thus derived were compared with the experimental data [17] on liquid He^4 based on neutron diffraction and X-ray scattering.

But as discussed above, in the case of the helium atoms in liquid He^4, the interaction potential is regarded as having hard repulsive core instead of soft ones as stipulated by Isihara [15]. However, Fourier transform of interaction of an interaction potential having a hard core cannot be evaluated. Moreover, if we only take the matrix element of the interaction potential, the effect of multiple scattering cannot be taken into account. Thus to take account of the effects of multiple scattering and also to use an interaction potential having a hard core, the Fourier transform of the interaction in Equation(4) U(q) should be replaced by the matrix elements of the reaction matrix t_q[Khanna et al].

Thus, we write the equation (4) as

$$\boxed{\varepsilon(q) = \frac{\hbar C q}{t_{00,00}^{1/2}}\left[t_q + \frac{\hbar^2 q^2}{4m^* \rho}\right]} \tag{15}$$

Where m^* is the effective mass of the bosons, $t_{00,00}$ is the ground-state reaction matrix and t_q is the reaction matrix for $q \neq 0$ states. The matrix elements of the reaction matrix t_q were calculated by Khanna et al. [10, 11] earlier using the theory of Brueckner and Sawada [18] and we have

$$t_q = t_{00,00}\frac{\sin qa}{qa} \tag{16}$$

Phukan et al. [12] have already used the ground-state reaction matrix $t_{00,00}$ for the interacting potential given by Eq.(1), as obtained from the work of Khanna and Das [13] and Khanna and Phukan [10,11] nhave the expression for $t_{00,00}$ when the interaction potential is of the type given by Eq.(2). Thus for the Gaussian equivalent of the Lennard-Jones potential,

$$t_{00,00} = \frac{\lambda^2 \hbar^2}{2m^* a^2 \rho} + 4\pi^{3/2}\varepsilon\left(\mu_R^3 - \mu_A^3\right) \tag{17}$$

And for the hard core followed by an attractive square well

$$t_{00,00} = \frac{\lambda^2 \hbar^2}{2m^* a^2 \rho} - \frac{4\pi\varepsilon}{3}(b-a)^3 \tag{17}$$

Equation (16) then gives

$$t_q = X_1 \frac{\sin qa}{qa} \tag{18}$$

where

$$X_1 = \left[\frac{\lambda^2 \hbar^2}{2m^* \rho a^2} + 4\pi^{3/2}\varepsilon\left(\mu_R^3 - \mu_A^3\right)\right] \tag{19}$$

For the potential of Equation (1) and

$$t_q = X_2 \frac{\sin qa}{qa} \tag{20}$$

where

$$X_2 = \left[\frac{\lambda^2 \hbar^2}{2m^* \rho a^2} - \frac{4\pi\varepsilon}{3}(b-a)^3 \right] \tag{21}$$

when the bosons are interacting via the potential given by Eq.(2)

With t_q thus calculated, the expression for the excitation energy ε(q) for the system of interacting bosons can be written from Eq.(15).

For finite temperatures and in the low momenta region, we have from Equations (3), (4) and (5), to a first approximation

$$S(q) = \frac{\hbar^2 q^2}{2m^* \varepsilon(q)} \left[1 + \frac{2kT}{\varepsilon(q)} \right] \tag{26}$$

For the Gaussian equivalent of the Lennard-Jones potential we thus obtain

$$S(q) = \frac{\hbar q X_1^{1/2} \left[1 + \frac{2kTX_1^{1/2}}{\hbar Cq \left\{ \frac{\hbar^2 q^2}{4m^* \rho} + X_1 \frac{\sin qa}{qa} \right\}^{1/2}} \right]}{2m^* C \left[\frac{\hbar^2 q^2}{4m^* \rho} + X_1 \frac{\sin qa}{qa} \right]^{1/2}} \tag{27}$$

And, for the hard sphere plus square well type of interactions we get

$$S(q) = \frac{\hbar q X_2^{1/2} \left[1 + \frac{2kTX_2^{1/2}}{\hbar Cq \left\{ \frac{\hbar^2 q^2}{4m^* \rho} + X_2 \frac{\sin qa}{qa} \right\}^{1/2}} \right]}{2m^* C \left[\frac{\hbar^2 q^2}{4m^* \rho} + X_2 \frac{\sin qa}{qa} \right]^{1/2}} \tag{28}$$

III. CALCULATIONS AND RESULTS:

Calculation for the structure factor at non zero temperatures T=0.4K, 0.6K and 0.8K as given by equation (27) and (28) have the results as shown in Table-I,II and III and figures 1, 2 and 3. In these calculations, we have the following values for the different parameters appearing equations (26), (27) and (28).

λ^2=33
μ_A^2=0.2206
μ_R^2=0.1103
a=2.1Å
b=4.0Å
m/m^*=1.6, 2.0

m=6.64x10^{-24}g
ε=14.11x10^{-16}erg
k=1.38x10^{-16}erg/deg

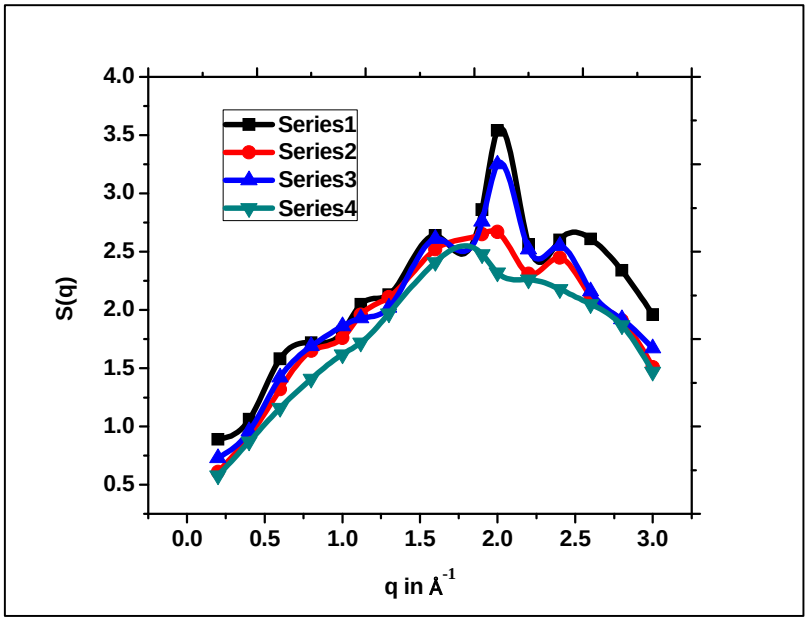

Fig1: Variation of S(q) with q at T=0.4K. Series 1 and 2 are for the Gaussian equivalent of Lennard Jones potential and series 3 and 4 are for hardcore followed by square well type of potential for m*/m=1.6 and 2.0 respectively.

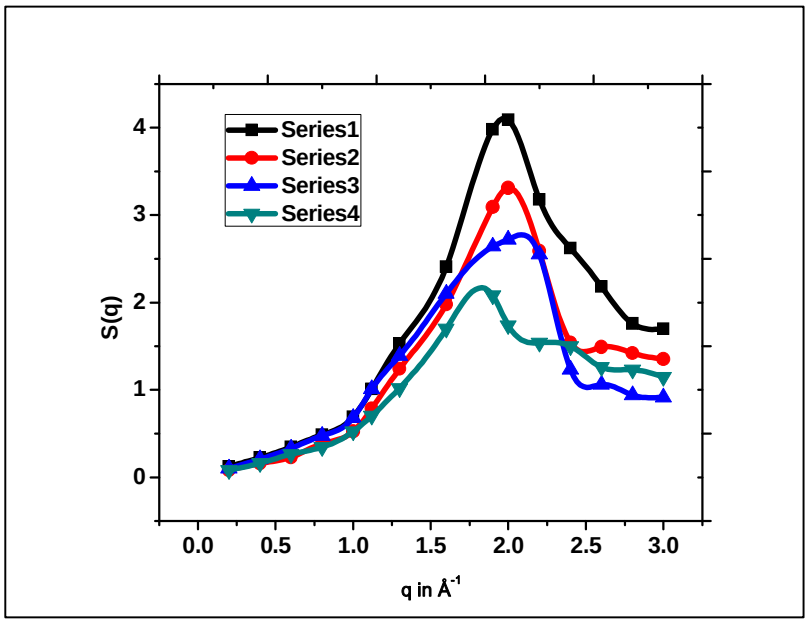

Fig2: Variation of S(q) with q at T=0.6K. Series 1 and 2 are for the Gaussian equivalent of Lennard Jones potential and series 3 and 4 are for hardcore followed by square well type of potential for m*/m=1.6 and 2.0 respectively.

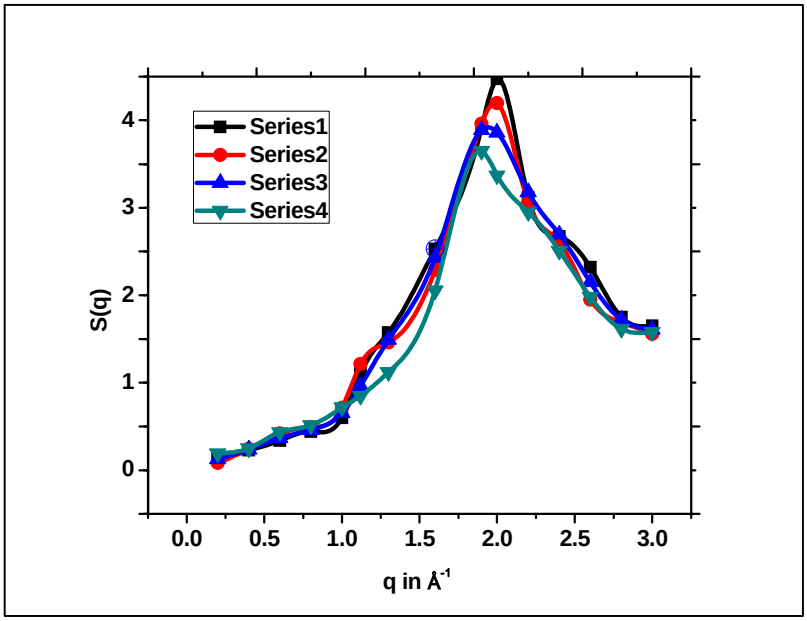

Fig3: Variation of S(q) with q at T=0.8K. Series 1 and 2 are for the Gaussian equivalent of Lennard Jones potential and series 3 and 4 are for hardcore followed by square well type of potential for m^*/m=1.6 and 2.0 respectively.

DISCUSSION

Fig 1 shows the variation of the structure factor S(q) with q for our systems of bosons at T=0.4K . Series (1) and (2) are for the case of hard spheres followed by the sum of two Gaussians and series (3) and (4) are for the case when the potential is hard core followed by an attractive square well, for m^*/m=1.6 and m^*/m=2.0 respectively. Similarly is the case with Fig2 (temp 0.6K) and Fig3 (temp 0.8K). From the graphs, it is seen that the peak in the S(q)-q graph is sharper and narrower when the potential is the Gaussian equivalent of the Lennard Jones potential. As structure factor indicates the degree of spatial order in the system, this result explains that when the particles interact with a potential having repulsive element after the hard core, the spatial ordering will increase. On the other hand, when the potential has a deeper attractive square well after the hard core the particles, after getting repelled by the hard core, get trapped in the attractive well and the particles will get spatially more delocalized, resulting in a broader peak.

Further, from the graph it is seen that the magnitude of the peak in S(q) decreases as m^*/m increases. Considering the fact that the peak in S(q)-q graph denotes the minimum in the excitation energy, we can infer from our results that, as m^*/m value increases i.e. when the particles become more and more repulsively interacting, the energy gap between the zero momentum state and the first excited state will be smaller.

In the experimental curve of Achter and Meyer [19] on structure factor of liquid He^4, peak of S(q) was at the q-value of $2Å^{-1}$. Our theoretical graphs also show the peak to occur exactly at $2Å^{-1}$in vicinity of this temperature for m^*/m=1.6, indicating interacting qualitative agreement between theory and experiment.

Henshaw [20] had shown that the temperature dependence of the spatial order in liquid He^4 undergoes a change in the vicinity of the Lambda transition temperature, T_λ. This result from experiment is reflected in our theoretical results (Fig1, 2 &3) when the S(q)-q graph enters the phonon region. There is a distinct sharp variation in the value of S(q).

Experiment conducted by V.F. Sears [17] and a host of the other workers show that a liquid He^4 is cooled towards T_λ. The spatial order shows a gradual increase as may be expected due to decrease in thermal disorder. Further cooling from the neighborhood of results in decrease T_λ results in decrease of spatial order. This result from experiment is also obtainable from our graphs where we find that the value of S(q) at 0.6K is higher than at T=0.4K.

The decrease in spatial order with decrease of temperature as shown in our graphs can be explained by admitting the phenomenon as a compensate of the occurrence of the Bose Condensate in liquid He^4. If on cooling a sizeable

fraction of He^4 atoms condense to a macroscopic state of definite momentum, then these atoms become spatially delocalized and the overall spatial order must decrease. In our case this is represented by the decrease in the value of S(q) with q in the phonon region. Thus the decrease in the spatial order may be attributed to the growth of a finite condensate fraction with lowering of temperature.

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