CHAPTER-I

REVIEWS OF THEORETICAL WORK ON SUPERFLUID $^4$HE
CHAPTER -1

EXPERIMENTAL OBSERVATIONS:

As mentioned in the general introduction liquid He II is the best example of quantum liquid. It is a Bose liquid which is well known for its very many interesting properties. It is found to remain as a liquid down to lowest attainable temperature under normal conditions. This is because of the fact that its zero point energy is large compared to the interparticle potential energy. A large zero point energy results due to its low mass

\[ p_{4\text{He}} = 0.145 \text{ gm/cm}^3 \].

It has been observed that $^4\text{He}$ undergoes a phase transition to the superfluid phase at a temperature of about 2.17°k. This is what is identified as the \( \lambda \) transition in liquid He-II. Below this temperature and at an applied pressure of 25 times the atmospheric pressure liquid He-II goes over to a solid phase. All these anomalous properties of liquid He-II (which is conventionally denoted by $^4\text{He}$) have given rise to overwhelming amount of experimental and theoretical activity over the past several years. For example, the measurement of its specific heat with temperature exhibits a singular behaviour as the temperature is lowered to \( T_{\lambda} \) and on further cooling it shows a \( T^3 \) variation. This singularity in the specific heat is generally thought to represent the onset of Bose condensation. The most spectacular property, that gives rise to its superfluid character, is its ability
to flow through fine capillary without experiencing any pressure drop. In any ordinary fluid there would have to be a pressure gradient through the tube since some force would be necessary to overcome the effect of shear viscosity. Since there is no pressure drop across the capillary in liquid $^4\text{He}$, it is natural to believe that liquid $^4\text{He}$ below the $\lambda$ transition point has no viscosity. One is therefore tempted to assume that zero viscosity is a property of superfluidity. An alternative way of measuring viscosity of superfluid $^4\text{He}$ was found to give a different result. The experiment was performed by plucking a violin string in a viscous fluid and observing the frequency of vibrations which is supposed to die away more rapidly in a viscous liquid than they would if the string were in vacuum. In such type of measurements the different in relaxation time would give a measure of viscosity. By measuring the viscosity of the superfluid $^4\text{He}$ in this way a finite result for the viscosity was obtained, which was inconsistent with the result of the superfluid flow through a capillary. The only way to understand this peculiar behaviour is to imagine that liquid $^4\text{He}$ in the superfluid phase is composed of two different kind of fluids those completely interpenetrate into each other. One is a normal fluid having finite viscosity and the other is a superfluid having no viscosity. This is how theoretically the two fluid model
for superfluid $^4$He was proposed, the hydrodynamics of the two-fluid model was worked out principally by L.D. Landau $^{2,3}$. If one thinks superfluid $^4$He as a degenerate Bose system, the normal fluid is to be identified with collective excitation out of the ground state, the first sound being one such excitation. As we have stated superfluid state may be characterised by the formation of Bose condensates. In order to maintain the superfluid character of liquid $^4$He, there must be some mechanism that prevents excitation out of the condensate, when it flows past the walls of the capillary tube. Following the two fluid model it can be worked out that an excitation of energy $\epsilon$ and momentum $K$ cannot be created in flow past an object unless the velocity $\nu$ of the object satisfies the relation $\nu \geq \epsilon/K$. If $\epsilon/K$ has some minimum value, then at velocities lower than that value, the condensate is a superfluid. One therefore has resistance to flow at velocity $\nu > \epsilon/K = \frac{K}{\sqrt{m}}$ (14) since the spectrum of the excited state of a perfect Bose gas is given by $\epsilon(\kappa) = \frac{K^2}{2m}$. From the above relation it follows that excited states are available at any velocity down to zero, since $K$ can have any value. This obviously means that perfect Bose gas is not a superfluid.

If one takes seriously the degenerate perfect Bose gas as a model of the superfluid, this must be modified in someway before it can serve as an adequate model for
superfluid Helium. Clearly this suggests that we have to abandon the relation $\epsilon(k) = k^2/2m$ as the energy spectrum of the excited states. Since the lowest excited energy states of the system was thought to be of the collective type a relationship of the form $\epsilon = SK$ was written down, where $S$ denotes the velocity of the sound. This very form of $\epsilon$ tells that the lowest excited states are the long wavelength phonons. Using this, the critical velocity was estimated to be given by $\nu > S$. In view of this fact there cannot be excitations at flow velocities less than $S$, so that for this part of the spectrum at least one can understand superflow. In other words, the picture of superfluid $^4$He that has emerged from the discussions made above is that of a condensate that constitutes the superfluid part, the excitations of which are not of the particle type but some kind of collective excitations of the system called phonons. The dispersion relation for the phonons was first worked by Landau $^2$, $^3$. Later on, in an attempt to account for the hydrodynamic properties such as the viscosity of the system, Landau and Khaltnikov $^20$ had to introduce a modification of the phonon dispersion relation by writing

\[ \epsilon = SK(1 - \gamma k^2), \]

where $\gamma$ was chosen to have the value $\approx 10^{-3} \text{ m}^{-2} \text{ cm}^{-2} \text{ s}^2$. As one notices this certainly indicates a departure from the linear dispersion. It turns out that the phonons alone
were not sufficient to explain the temperature dependence and the absolute values of thermodynamic quantities like the specific heat. This is how it led to modify the above dispersion relation for shorter wavelength (larger $K$). A relation of the type was written down

$$\varepsilon = \Delta + \frac{(K-K_0)^2}{2\mu^2}$$

(1.3)

where $K_0$ denotes the value of the momentum at which the function $\varepsilon$ has a minimum value equal to $\Delta$. Eq. (3) is valid in the neighbourhood of $K_0$. The exact value of the parameter $\Delta$ and $K_0$ were found by neutron scattering experiments which gives $K_0/\hbar \approx 2 \times 10^{-1}$, $\Delta \approx 0.1 K$ and $\mu \approx 0.16 m_{\text{He}}$. The energy spectrum of liquid $^4\text{He}$ is graphically shown in Fig. 1. In this graph the excitations in the region of parabolic minimum are given the name rotons. The parameter $\mu$ appearing in equation (1.3) is usually called as the effective mass of the roton. The new development in the excitation spectrum of liquid $^4\text{He}$ is of more microscopic nature and hence it serves as a more powerful theory than the two fluid model. It still forms a phenomenological theory because the concepts and parameters those are involved in such kind of theory are obtained from experiments rather than from the microscopic interaction between the atoms. Feynman$^{21}$ and Feynman and Cohen$^{22}$ attempted to obtain a more microscopic model and put Landau's idea in a firmer theoretical basis. The observation of the excitations in liquid $^4\text{He}$ was first made by Palevsky et al.$^{38,39}$
Fig. 1. Plot of Excitation energy $\varepsilon(k)$ versus momentum $k$. 
Henshaw and Woods 41, using inelastic neutron scattering. Subsequent measurements on the detailed shape of the energy-momentum dispersion curve for the excitation spectrum were done by several workers 38-48. These experiments confirmed Landau's essential idea and hence proved the basis for more detailed microscopic theories.

The main results of the Feynman-Kohen theory is to express the excitation spectrum $\varepsilon(k^2)$ as

$$\varepsilon(k^2) = \frac{\kappa^2 k^2}{2m} s(k^2)$$

where $s(k^2)$ denotes the static structure factor of liquid $^4$He. The static structure factor is nothing but the Fourier transform of the pair correlation function; as such, it gives the information about the correlated motion of particles in the system. $s(k^2)$ can be determined experimentally by knowing the intensity of the inelastically scattered neutron or x-rays. The function $s(k^2)$ is such that for large $k$, it tends to be unity, and for small values of $k$, it goes to zero linearly with $k$ at $T=0$, corresponding to the fact that for large distances the correlation among the particles disappear. This is found to have a maximum at values of $k \approx 2\pi/\lambda$, where $\lambda$ is the average inter-particle distance. The form of $s(k^2)$ is shown in figure (2). Following this, the resulting form for $\varepsilon(k^2)$ versus $k^2$ is obtained which agrees with the plot shown in Fig.1. From this figure one notices that the linear portion of the graph (the graph in the region of small $k$) corresponds to the phonon part of the spectrum. Near the region of
Fig. 2. Plot of static structure function $S(k)$ versus momentum $K (\AA^{-1})$. 
minima in the curve (which corresponds to the values where \( S(\mathbf{R}) \) has a maximum), \( \in (\mathbf{R}) \) very well fits with the form given by equation (1.3). Finally for \( \mathbf{k} \rightarrow 0, \in (\mathbf{R}) \Rightarrow \frac{K^2}{2m} \), meaning that the spectrum goes over to that of the free particles.

**THEORETICAL FORMULATIONS:**

A rigorous derivation of the energy spectrum of liquid \( ^4\text{He} \) has not been so far obtained theoretically although a large number of model calculations exist to explain the spectrum over entire momentum range. We shall describe a simple model which gives the energy spectrum that has properties similar to those described above. This is the calculation due to Bogoliubov \(^{15}\) which is based on the picture of a non ideal Bose gas of particles with zero spin. The particles in the system are assumed to interact among themselves weakly. The Hamiltonian of the system is written in second quantised form as

\[
H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_1',\mathbf{k}_2'} V_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_1',\mathbf{k}_2'} a_{\mathbf{k}_1}^+ a_{\mathbf{k}_2} a_{\mathbf{k}_2'} a_{\mathbf{k}_1'}
\]

(1.5)

where \( \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_1', \mathbf{k}_2' \) are the momenta of the interacting particles, \( V_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_1',\mathbf{k}_2'} \) is the Fourier transform of the interparticle potential which is a measure of the coupling strength. In equation (1.5) \( a_{\mathbf{k}}^+, a_{\mathbf{k}} \) are the creation and annihilation operators such that

\[
\left[ a_{\mathbf{k}}, a_{\mathbf{k}'}^+ \right] = \delta_{\mathbf{k},\mathbf{k}'}
\]

(1.6)

and so on. Considering the fact that the momentum is
conserved one writes \( \vec{k}_1 + \vec{k}_2 = \vec{k}'_1 + \vec{k}'_2 \).

since the system is assumed to be in the neighbourhood of temperature \( T = 0 \), it is considered to be a degenerate one. Therefore the values of the momenta that the particles can have will be very small. As a result, the momentum transferred in a collision has to be small. Since the interparticle potential is weak the ground state of the system would be the one in which the particles are assumed to form Bose condensates. In the condensed state the momentum transferred among the particles is zero. If \( N_0 \) be the total number of particles in the system, \( N \) is the average number of particles in the ground state, then \( (N-N_0) = \eta \) should be the number of particles in the excited state. However, the number is supposed to be very small. For sufficiently low temperatures, the interaction is being treated as independent of the momentum transfer and the creation and annihilation operators at zero momentum transform are treated as ordinary numbers approximately equal to \( \sqrt{N} \).

Under the above situation, the Hamiltonian may be written as

\[
H = \sum_{\mathbf{K}} \epsilon_{\mathbf{K}} \hat{a}_{\mathbf{K}}^{\dagger} \hat{a}_{\mathbf{K}} + \frac{1}{2} V_{0} N^2 + N_0 \sum_{\mathbf{K}} V_{\mathbf{K}} \hat{a}_{\mathbf{K}}^{\dagger} \hat{a}_{\mathbf{-K}}^{\dagger} \hat{a}_{-\mathbf{K}} \hat{a}_{\mathbf{K}} \\
+ \frac{1}{2} N_0 \sum_{\mathbf{K}} V_{\mathbf{K}} (\hat{a}_{\mathbf{K}}^{\dagger} \hat{a}_{\mathbf{-K}}^{\dagger} + \hat{a}_{\mathbf{-K}} \hat{a}_{\mathbf{K}}) 
\]

where \( \hat{a}_{\mathbf{K}}^{2} + \sum_{\mathbf{K} \neq \mathbf{K}'} \hat{a}_{\mathbf{K}}^{\dagger} \hat{a}_{\mathbf{K}'} = N \) \hspace{1cm} (1.7)

and \( V_{\mathbf{K}} = V_{\mathbf{-K}} \).

The above Hamiltonian is correct to second order in the operators \( \hat{a}_{\mathbf{K}}^{\dagger} \) and \( \hat{a}_{\mathbf{K}}^{\dagger} \). From these discussion one finds that it should be adequate to describe a gas of weakly
interacting bosons near the absolute zero of temperature by means of a Hamiltonian given in eq. (1.7).

The very Hamiltonian is such that it does not conserve particle number. In order to diagonalise this Hamiltonian we introduce the canonical transformation as defined as

\[ a_{k} = u_{k} a_{k}^{\dagger} + n_{k} a_{-k}^{\dagger} \]
\[ a_{k}^{\dagger} = u_{k} a_{k}^{\dagger} + n_{k} a_{-k}^{\dagger} \]  \hspace{1cm} (1.8)

where \( a_{k} \) and \( a_{k}^{\dagger} \) are quasi(pseudo) particles annihilation and creation operators and they obey same commutation relation as the particle annihilation and creation operators \( [a_{k}, a_{k}^{\dagger}] = \delta_{k, k'} \). In equation (1.8) \( u_{k} \) and \( n_{k} \) are such that

\[ u_{k} = u_{-k} \]
\[ n_{k} = n_{-k} \]
and
\[ u_{k}^{2} - n_{k}^{2} = 1 \]  \hspace{1cm} (1.9)

with this the Hamiltonian gets reduced to the form

\[ H = \sum_{k} \left( E_{k} + N n_{k}^{2} \right) \left( u_{k}^{2} a_{k}^{\dagger} a_{k}^{\dagger} + n_{k}^{2} a_{-k}^{\dagger} a_{-k}^{\dagger} \right) \]
\[ + \sum_{k} N n_{k} u_{k} a_{k}^{\dagger} a_{k}^{\dagger} \left( a_{k}^{\dagger} a_{k}^{\dagger} + a_{-k}^{\dagger} a_{-k}^{\dagger} \right) \]
\[ + \sum_{k} \frac{N}{2} \left( u_{k}^{2} + n_{k}^{2} \right) + \frac{N}{2} \left( u_{k}^{2} + n_{k}^{2} \right) \]
\[ \times \left[ \delta_{k, k'} \left( a_{k}^{\dagger} a_{k}^{\dagger} + a_{-k}^{\dagger} a_{-k}^{\dagger} \right) \right] + V_{0} N^{2} \]  \hspace{1cm} (1.10)

This can be cast into a diagonalised form by setting the
coefficient of $\alpha_{R^2}^+$ (or of $\alpha_{-R^2}^+$) to zero.

That amounts to having

$$E_{R^2} \alpha_{R^2} \cdot \alpha_{R^2}^* + \frac{1}{2} N v_{R^2} \left( \alpha_{R^2}^2 + \alpha_{R^2}^* \right) = 0$$

(1.12)

and

$$\alpha_{R^2} \cdot \alpha_{R^2}^* = \frac{E_{R^2} - N v_{R^2}}{\left[ (E_{R^2} + N v_{R^2})^2 - N^2 v_{R^2}^2 \right]^{1/2}}$$

Now the Hamiltonian becomes

$$H = U + V_0 N^2 + \sum_{R^2} E_{R^2} \alpha_{R^2}^+ \alpha_{R^2}^*$$

(1.13)

where

$$U = \sum_{R^2} \left( \frac{E_{R^2}}{N} + N v_{R^2} \right) \left( \alpha_{R^2} \cdot \alpha_{R^2}^* \right)$$

denotes a constant shift in energy.

$$T_{R^2} = E_{R^2} + N v_{R^2}$$

and

$$E_{R^2} = T_{R^2} \left( \alpha_{R^2} \cdot \alpha_{R^2}^* \right) + N v_{R^2} \alpha_{R^2} \cdot \alpha_{R^2}^*$$

is the energy of the quasiparticle. Using the expressions $\left( \alpha_{R^2} \cdot \alpha_{R^2}^* \right)$, $\left( \alpha_{R^2} \cdot \alpha_{R^2}^* \right)$ and $\left( \alpha_{R^2} \cdot \alpha_{R^2}^* \right)$

$E_{R^2}$ reduces to the form

$$E_{R^2} = \left( E_{R^2} + 2 E_{R^2} N v_{R^2} \right)^{1/2}$$

(1.14)

From this we see that for small $K$ values, i.e., for low momenta $E_{R^2} \rightarrow \left[ 2 N v_{(0)} E_{R^2} \right]^{1/2} = \kappa \left( \frac{N v_{(0)}}{m} \right)^{1/2} \approx S \kappa$ (1.15)

where $S$ may be interpreted as the sound velocity and

$$S = \left( \frac{N v_{(0)}}{m} \right)^{1/2}$$

This is why one justifies calling the quasiparticles as the phonons. One further sees that for large momenta $K \rightarrow \infty$

$$E_{R^2} \rightarrow E_{R^2} = \frac{K^2}{2m}$$

(1.16)
Therefore in limit of \( v \rightarrow \infty \) the quasiparticles have the character of single particle excitations. Though the above picture does not describe the entire region of the spectrum but still it gives a very good fit in the large and small momentum region. In the intermediate momentum region, if one writes

\[
E_R \approx \varepsilon_R + 2N\sqrt{\varepsilon_R}
\]

the factor \( 2N\sqrt{\varepsilon_R} \) may be interpreted as energy gap \( \Delta \). This way one may get a feeling of the roton branch of the excitation spectrum to which a nonzero excitation energy \( \Delta \) was associated. Thus the whole spectrum of excitations consists of two separate branches, the phonon branch describes a rotation free motion and the roton branch describing rotational motions of the system. However, both the type of excitations have to be considered as two parts of one and the same excitation energy-momentum curve \( E(\mathbf{k}) \) and there is a continuous transition from one to the other form of the roton part of the energy. This very aspect of the excitation spectrum has not yet been successfully investigated theoretically. Besides, the form of roton part of the spectrum as proposed by Landau has not been obtained from any microscopic theory till today. There have been of course several investigation 26-37 about the nature of collective excitations of superfluid helium and
in such studies many assumptions have been made. In the absence of tractable microscopic theory of strongly interacting Bose system, many of these assumptions have not been given on a firm theoretical basis. Perturbative calculations of Bose systems using Green’s function formalism of many body systems have been carried out by Balitsky, Hugenholtz and Pines and by Hohenberg and Matin etc. In these theories one encounters tremendous difficulties in evaluating single particle self energies. Besides in most cases some unphysical features like the violation of conservation laws are found to occur in these calculations. Furthermore, calculations beyond the well known Bogoliubov approximation are tedious due to the appearance of spurious divergences. However, as far as the properties near the phase transition of normal Helium are concerned, a theory was proposed by Landau, according to which the free energy of the system in the superfluid state was expanded as a polynomial in terms of its order parameter. The order parameter is such that for temperature greater than the critical temperature \( T_c \), the order parameter vanishes and it goes to zero continuously as \( T \to T_c \). The Landau theory was meant to be applicable to the second order phase transitions as is the case with liquid \(^4\)He. For superfluid \(^4\)He the microscopic wave function \( \Psi \) of the system is treated as the order parameter. The superfluid number density \( \rho_s \) is expressed as

\[
\rho_s = m |\Psi|^2
\]  
(1.18)
Since the original theory of Landau did not have a term to explicitly account for the spatial variation of the order parameter $\psi$, it was subsequently modified by Pitaevskii and Landau by the addition of a factor proportional to $\left| -i \pi \nabla \psi \right|^2$ into the expression for free energy. This very inclusion is equivalent to having a kinetic energy term in the free energy. One therefore deals with the expansion of the free energy density $f_s(\nabla^2)$ which is written as

$$f_s(\nabla^2) = f_n(\nabla^2) + \alpha |\psi|^2 + \beta |\psi|^4 - \frac{\hbar^2}{2m} \left| \nabla^2 \psi \right|^2$$

(1.19)

In this equation $f_n(\nabla^2)$ denotes the free energy density corresponding to the normal state, the parameters $\alpha$ and $\beta$ are the temperature dependent coefficients, which are characteristic constants of the system in its superfluid state and $m$ is the mass of the helium atom. Following (1.19) one obtains the total free energy density of the system as

$$F_s = \int f_s(\nabla^2) \, d\nabla$$

(1.20)

using a variational treatment for $f_s$ with respect to $\psi (\nabla^2)$ one arrives at the following equation of motion for $\psi$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + \alpha |\psi|^2 + \beta |\psi|^4 \psi = 0$$

(1.21)
This is a non-linear Schrödinger equation for $\psi$. If one ignores the spatial variation of $\psi$, from the minimisation of $f_5$ with $\psi$, it follows that

$$\alpha = A(T - T_c)$$

where $A$ is a positive constant and $\beta$ is also a constant which depends on $T_c$. The phenomenological constants $\alpha$ and $\beta$ are determined from a fit with the experimental data of the specific heat and superfluid density $\rho_s$ around $T_c$. The parameter $\alpha$ is such that it is negative for $T < T_c$. Writing down the non-linear Schrödinger equation (1.21) in dimensionless form after reducing it to a one-dimensional geometry one obtains the coherence length

$$\xi(T) = \left[ \frac{\hbar^2}{2m|\alpha|} \right]^{1/2} = \frac{\hbar}{\sqrt{2mA(T_c - T)}}^{1/2} (1.22)$$

Physically, the coherence length defines a natural scale of length for the spatial variations of the order parameter. As we can see from above $\xi(T) \to \infty$ when $T \to T_c$. An estimation of $\xi(T)$ shows that $\xi(T)$ except at the critical point is comparable to the inter-atomic spacing where the Pitaevskii Landau theory breaks down. This deficiency is due to the fact that the Pitaevskii Landau theory does not take into account fluctuation effects which are supposed to be very large near $T_c$. An improvement over this theory was later done by Khalatnikov trying to incorporate fluctuation effects into the theory. With this he succeeded in deriving the
As regards the theoretical study on liquid superfluid $^4\text{He}$ is concerned there has not been much progress from microscopic point of view other than what we have already discussed earlier. However, there were several interesting experiments $^{38-49}$ about which we have mentioned, had led to accurate measurement of $S(k)$. An important observation was made on the property of superfluid $^4\text{He}$ in the year 1970 by Cowley and Woods $^{44}$ following their famous experiment on superfluid $^4\text{He}$ using inelastic scattering of slow neutrons of a very high flux those were available from the NRU reactors of Chalk River in Canada. This very experiment of Cowley and Woods showed an extra peak in the intensity of the scattered neutrons in addition to the one known earlier. The new peak which obviously refers to a new branch of excitations in superfluid $^4\text{He}$ was attributed to multphonon/pair excitations of the system. Speaking in this language the first peak is being identified with the one phonon excitation of the system. The intensity of the scattered neutrons which is nothing but is differential scattering cross section is directly related to the dynamic structure factor $S(k^2,\omega)$ of the
system through the formula
\[
\frac{d^2 \mathcal{G}}{d \Omega \, dE} = \frac{G_0}{4 \pi \hbar} \frac{Q'}{Q'_0} \, \mathcal{S}(\mathbf{k}, \omega) \tag{1.23}
\]

where \(d \Omega\) is the solid angle of the scattered beam and \(dE\) the corresponding energy interval. \(Q'\) and \(Q'_0\) represent the incident and scattered neutron beams respectively. \(\mathbf{k}\) is the transferred momentum and \(G_0\) is the scattering cross section for isolate bound atom and \(\mathbf{k} \omega\) is the energy transfer in the scattering process. \(\mathcal{S}(\mathbf{k}, \omega)\) is defined as
\[
\mathcal{S}(\mathbf{k}, \omega) = \frac{1}{N \pi} \, \mathcal{F}(\mathbf{k}, \omega) \tag{1.24}
\]

where \(\mathcal{F}(\mathbf{k}, \omega)\) is called the density-density response function. This is given by
\[
\mathcal{F}(\mathbf{k}, \omega) = - i \int_{-\infty}^{\infty} \, d \varepsilon \, e^{i \omega \varepsilon} \left\langle \left| T \frac{\mathbf{\rho}(\varepsilon) \rho^{(0)}(\varepsilon)}{\mathbf{k}^2} \right| \right\rangle \tag{1.25}
\]

where \(\mathbf{\rho}(\varepsilon)\) is the density fluctuation operator
\[
\mathbf{\rho}(\varepsilon) = \sum_{\varepsilon = 2}^{N} \, e^{-i \mathbf{k} \cdot \mathbf{r}_\varepsilon(\varepsilon)} \tag{1.26}
\]

Therefore, theoretically there were several attempts to explain the intensity of the scattered neutrons through determination of \(\mathcal{S}(\mathbf{k}, \omega)\). After the discovery of the new mode of excitation in superfluid liquid \(^4\)He its phonon dispersion curve was measured. This was done by
looking at the values of $\omega_k$ at the peak positions of $S(\mathbf{k}, \omega)$ for a fixed value of the momentum transfer $\mathbf{k}$, with the determination of the new phonon dispersion curve, a large number of research workers got interested to explain the spectrum theoretically. In most of these works the emphasis was on evaluation of a good $S(\mathbf{k}, \omega)$ of the system. The dynamic structure function defined through equation (1.24) and (1.25) can be put into the form:

$$S(\mathbf{k}, \omega) = \sum_n \left| \left( \frac{\partial}{\partial \mathbf{k}_n} \right)_n \right|^2 \delta(\omega - \omega_n)$$

(1.27)

where $\omega_n = E_n - E_0$, $E_n$ being the energy corresponding to the $n^{th}$ excited state of the system.

From the right hand side of equation (1.27) it is noticed that $S(\mathbf{k}, \omega)$ consists of the contribution from the various excited states of the system, the excited state characterised by $n = 1$ corresponds to one-(pair/phonon) excitation, and that characterised by $n = 2$ correspond to two pair/phonon excitations of the system and so on.

Since there were mathematical difficulties in evaluating the contributions coming from the excited states, other than $n = 1$ in equation (1.27), there were attempts to explain the phonon dispersion curve using a polynomial fitting formula. To fit the experimental data corresponding to the one phonon part of the dispersion curve the expression for $\omega_k$ was found to be represented.
by the formula

$$\omega_{\mathbf{k}} = C_{\mathbf{k}} [1 - \gamma k^2 - \delta k^4]$$  \hspace{1cm} (1.28)$$

where the constants \(\gamma\) and \(\delta\) were estimated from fitting with the result obtained by Woods and Cowley (1970)

$$\gamma = 0 \pm 2 \times 10^{-36} \text{ cm}^{-2} \text{ s}^{-2}$$

$$\delta = 2.4 \pm 0.3 \times 10^{-35} \text{ cm}^{-4} \text{ s}^{-4}$$

The above expansion was tried to be explained theoretically by Feenberg 1971 and Gould Wong (1971) but they have failed to explain. The above expansion gave rise to a very good fit for values of \(K \leq 1 \text{ A}^{-1}\)

In view of the Feynman coherence structure function formula the one phonon static structure factor measured by Woods and Cowley was written as

$$S(\mathbf{k}^2) \Rightarrow Z(\mathbf{k}^2) = \frac{h k}{2 \omega_c} [1 - Z_2 k^2 - Z_4 k^4]$$  \hspace{1cm} (1.29)$$

where

$$Z_2 = 1.5 \pm 0.2 \text{ A}^2$$

$$Z_4 = -0.9 \pm 0.2 \text{ A}^4$$

But Hallock's experimental observation for static structure function was a refined one. The above fitting formula for \(Z(\mathbf{k}^2)\) does not fit with Hallock's observation. Also the expression for \(\omega_{\mathbf{k}}\) as given by equation (1.28) was inadequate to explain the phonon
dispersion over the entire region of momentum transfer which extends up to \( \kappa = 2 \cdot 5 \AA^{-1} \). This was due to the fact, that the region \( \Delta \kappa^0 \kappa \leq 2 \cdot 5 \AA^{-1} \) was assumed to have contributions arising not only from one-phonon but also from two and higher phonon excitations. It was therefore assumed that the total static structure factor as measured by Hallock has now a component coming from two and higher phonon/pair excitations which is being described by \( S_{\Pi}(\kappa^2) \).

Considering \( S_{\Pi}(\kappa^2) \) to be represented by the formula

\[
S_{\Pi}(\kappa^2) = G_{\Pi} \kappa^4 + G_{\Pi} \kappa^6
\]

the expression for \( S(\kappa^2) = Z(\kappa^2) + S_{\Pi}(\kappa^2) \) becomes such that the coefficient of \( \kappa^4 \) is related to \( Z_2 \) and \( \gamma \). It is interesting to note that \( S_{\Pi}(\kappa^2) \) as given by equation (1.30) is seen to contribute to order \( \kappa^4 \) and higher power of \( \kappa \). Because of this modified expression for \( S_{\Pi}(\kappa^2) \) the formula for \( \omega(\kappa) \) got changed and with this one could only achieve a fairly good fit up to value \( \kappa \leq 3 \AA^{-1} \). The discrepancy in the intermediate momentum transfer region \( 0.3 \kappa < \kappa < 2 \cdot 5 \AA^{-1} \) has been interpreted as due to not properly accounting for two-phonon/pair excitation contributions. To explain the experimental data in the intensity of the scattered neutrons in the momentum transfer region \( 0.5 \AA^{-1} \kappa < \kappa < 2 \cdot 4 \AA^{-1} \).
where the double peak structure in $S(k, \omega)$ has been usually observed. There were some interesting calculation by Iwamoto, Pitaevskii, and Zawadowski et al. All of them try to consider the effect of roton-roton interaction in the shape of the intensity distribution of the scattered neutrons. This study tells that such interactions may have significant effect on the shape. In particular the calculations by Zawadowski et al. shows a qualitative agreement with the observed neutron scattering data. Seda et al. try to explain the scattering data by satisfying the zeroth and first moment theorem. Approximately $S_{II}(k, \omega)$ by $S_{II}(k)$ $S(\omega - \omega_{2}(k))$, they are able to obtain $S_{II}(k)$ by using the results for the observed one phonon and multiphonon peak frequency. This is also of qualitative nature.

The various theoretical methods we have discussed above which have been used for the study of excitation spectrum in superfluid give rise to only a qualitative understanding of the same. As regards underlying approximations are concerned, they have not been given on a firm theoretical basis. In order to understand them from a microscopic point of view Wong and Gould have performed a microscopic analysis of the long wavelength excitations in superfluid helium based on the dielectric formulation of a dilute Bose gas at zero
temperature. In their study they have emphasised on the role of the interaction and the effects of the condensate. The advantage of the formulation is that it enables them to make explicit calculation beyond the Bogoliubov approximations with relative ease and without spurious divergences. Local number conservation is incorporated into their formulation by means of the generalised ward identities. The dynamic structure function evaluated by these authors is conveniently separated into three parts, i.e. one-phonon term which exhausts the sum rule, a backflow term and a background term. The backflow contribution to the static structure factor leads to the breakdown of the one-phonon Feynmann relation of order $v_0^3$. The two-phonon excitation contribution to $S(x,\omega)$ gives rise to a broad background in their theory. Although their approach proves to be quite instructive in improving phenomenological results but the studies are not directly applicable to superfluid $^4$He. More extensive study of this kind has been later on carried by Wong, Family and Gould $^{34,35}$. In a subsequent paper Wong $^{37}$ has tried to explain the inelastic scattering data in the deep inelastic scattering region by assuming that the dominant contribution in the region comes from two-phonon excitation. However to obtain a fit with the experimental data in the above region he has introduced two parameters in an adhoc manner in...
order to account for the contribution arising due to the background and that resulting because of the approximation used in his theory. In the high frequency region the $S(k^2, \omega)$ of his theory is found to vary as $k^4/\omega^{7/2}$ for a Bose class of particles. Family has also arrived at a similar behaviour for $S(k^2, \omega)$ in the large $\omega$ region following a diagramatic perturbation theory for the problem. The peak at $\omega \approx 2.5k$ still remained unexplained in the theory given by Wong. Besides Wong also could not succeed to explain the experimental data in the relatively low energy region. The aim of this thesis is partly to explain the inelastic neutron scattering data both in the low and high energy region, theoretically. We in fact have succeeded in doing so. Our theory, which essentially aims at obtaining a fairly accurate determination of the two phonon/pair contribution to $S(k^2, \omega)$ is able to reproduce a peak which corresponds to the broad peak observed in the experiment. This has been discussed in detail in chapter-XII of this thesis.
STUDY OF TWO-PHONON EXCITATION IN SUPERFLUID $^4$He
II.A  CALCULATION OF CONTRIBUTION OF TWO PHONON EXCITATION TO DYNAMIC STRUCTURE FACTOR

In the chapter-I we have given a review of the theoretical development in superfluid $^4$He. In this chapter we try to explain the neutron scattering data due to Cowley and Woods$^{45,47,48}$ on this system in the deep inelastic scattering region. As we discussed earlier the inelastic scattering experiments by Cowley and Woods from superfluid $^4$He showed for the first time the presence of a broad secondary peak in the high energy transfer region for values of momentum transfer $k < 1.8 \text{ } \text{ Å}^{-1}$. For values of $k$ larger than $1.8 \text{ } \text{ Å}^{-1}$ the second peak is found to disappear. It may be mentioned that the peak around the one-phonon frequency is identified as the one-phonon excitation of the system. Since the position of the broad peak was observed at a frequency close to almost twice the one phonon frequency it was interpreted that this perhaps corresponds to the two-phonon excitations of the system. To explain the intensity of the scattered neutrons in high energy transfer region, Wong$^{37}$ evaluated the two pair/phonon excitation contribution, $S_{II}(k, \omega)$ to the dynamic structure factor $S(k, \omega)$ which has been defined through eq. (12.27). He obtained
a \frac{k^4}{\omega^{7/2}} behaviour for \Sigma_{\Pi}(\overrightarrow{K},\omega) in the limit of very large \omega for a neutral Bose system, whereas for the charged Bose system his theory exhibited a \frac{k^4}{\omega^{7/2}} variation. Such type of behaviour was found to be an universal feature of both Fermi and Bose systems (that is irrespective of what statistics the particles of the system obey). This was rather dependent on the nature of the interparticle potential in the system. Family\textsuperscript{36} had arrived at a similar variation by looking at the high frequency behaviour of the density-density response function of the system, following a diagramatic perturbation theory.

The expression for \Sigma_{\Pi}(\overrightarrow{K},\omega) obtained by Wong was such that in order to obtain a good fit with experimental data in the tail portion of the high frequency transfer region he had to introduce two parameters into his theory. As we have mentioned, one of these parameter was meant to account for the contribution arising due to the background and the other to account for the approximation used therein. Although Wong's calculation give rise to a reasonable good fit in the high frequency transfer region, it shows a rising up tendency as one comes to relatively low frequency side of the intensity curve. In other words, the low frequency part of the intensity curve is not at all reproduced following Wong's theory. This being
the situation, obviously there is no hope of getting
the secondary peak from Wong's theory. We have
succeeded in getting rid of both these deficiencies
using a procedure which enables us to calculate \( S_{\Pi}(\mathbf{k}, \omega) \)
with great accuracy. Our theory in fact is free from
any adjustable parameter, as introduced by Wong. We
start with the equation of motion for the density
fluctuation operator and use its result to evaluate
the two-pair/phonon contribution to \( S_{\Pi}(\mathbf{k}, \omega) \). From
our calculation, we find that in the limit of large
\( \omega \), \( S_{\Pi}(\mathbf{k}, \omega) \) for superfluid \( ^4 \! He \) goes as \( k^2/\omega \) instead of having the variation \( k^4/\omega^{7/2} \) as obtained
by Wong\(^{37} \) and Family\(^{36} \). Under suitable approximation
the interesting feature of our theory is that it
reproduces a peak in the intensity versus \( \omega \) curve
in the high energy region. We have evaluated \( S_{\Pi}(\mathbf{k}, \omega) \)
in the high energy transfer region for the value of
momentum transfer \( k \approx 0.6 \text{ \AA}^{-1} \), \( k \approx 0.8 \text{ \AA}^{-1} \).
In all cases we find peaks in \( S_{\Pi}(\mathbf{k}, \omega) \) which are
very close to the values of \( \omega \) at the positions
of the second peak, that are observed in the neutron
scattering experiments\(^{44} \) that is why we identify the
experimentally observed secondary peaks with those
corresponding to the two-phonon excitations.

**Theoretical Calculation:**

We recall the definition of \( S_{\Pi}(\mathbf{k}, \omega) \) as given
by Eq. (1.27). In this equation the sum over \( \eta \) refers
to the various excited states of the many body system
and \( \omega_{n,0} \) which is equal to \( E_n - E_0 \) denotes the
excitation energy. Since the one-phonon excitation
contribution to \( S_k(w) \) correspond to the excited state
\( n = 1 \), where we shall not be concerned with the
contribution to \( S_k(w) \) arising from \( n = 1 \). This
means we primarily confine ourselves to the contribution
coming from \( n = 2 \) which we here denote by \( S_k(w) \).

As we know, for a fixed value of the momentum transfer,
the one phonon excitation spectrum persists up to some
values of \( \omega \). Beyond this value the two phonon exca-
tation contribution is likely to start. Since we
assume that the peak in the high energy transfer
region of \( S_k(w) \) is dominantly contributed by the
two-phonon (pair) excitations, we justify in retaining
the contribution due to \( n = 2 \) only if the dominant
contributions, this means equation (1.27). In order
do the evaluation of \( S_k(w) \) we consider the
equation of motion for the density fluctuation operator
\[
\frac{d}{dt} \rho_k^+(t) = \left[ \rho_k^+, \hat{H} \right]
\]
(2.1)

where the many particle Hamiltonian \( \hat{H} \) is written in
terms of the density fluctuation operator as
\[
\hat{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{q \neq 0} \frac{V(q)}{q} \left( \rho_q^+ \rho_q - N \right)
\]
Following (2.1) and (2.2) we obtain

\[
\hat{\rho}_k^+ = -\sum_{i=1}^{N} \left( \frac{2}{m} \left( \frac{\mathbf{k} \cdot \mathbf{p}_i}{m} - \frac{\mathbf{k}^2}{2m} \right) \right) e^{-i \mathbf{k} \cdot \mathbf{r}_i} + \sum_{q \neq 0}^{} \frac{2}{m} \mathbf{k} \cdot \mathbf{q} \cdot \tilde{V}(\mathbf{q}) \cdot \hat{\rho}_{-q}^+ \tag{2.3}
\]

where \( \tilde{V}(\mathbf{q}) \) denotes the Fourier transform of the inter-particle potential, and \( m \) is the mass of helium atom. We choose the potential acting between any pair of atoms in the liquid to be of short range type that is

\[
\tilde{V}(\mathbf{q}) = \frac{4\pi \hbar}{m} \delta(\mathbf{q})
\tag{2.4}
\]

\( b \) being the scattering length. Since the first term in (2.3) is proportional to a single density fluctuation operator it does not contribute to matrix element \( (\hat{\rho}_k^+)_{10} \) when averaged over the states \( |1\rangle \) and \( |2\rangle \).

In the Heisenberg representation the time dependence of the density fluctuation operator \( \hat{\rho}_k^+(t) \) is taken out and taking its matrix element between the states \(|1\rangle \) and \(|10\rangle \) can be written as

\[
(\hat{\rho}_k^+(t))_{10} = (\hat{\rho}_k^+(0))_{10} e^{-i \omega_{no} t}
\tag{2.5}
\]

and

\[
(\hat{\rho}_k^+(t))_{10} = -\omega_{no}^2 (\hat{\rho}_k^+(0))_{10} e^{-i \omega_{no} t}
\tag{2.6}
\]

Thus if the state \( n = 2 \) is considered and comparing

\[2058 \neq 6\]
Using the inverse Fourier transform for $\mathcal{V}(\mathbf{q})$ and the expression for $f_{j}^{\dagger}$ in (2.7) the expression for $(f_{k}^{\dagger})_{20}$ in $\gamma$ space can be written after interchanging $i$ and $j$ as

$$
(f_{k}^{\dagger})_{20} = -\frac{1}{2a} \left< 2 \left| \frac{1}{m \omega_{20}^{2}} \sum_{i \neq j} \mathcal{V}(\mathbf{\hat{q}}_{ij}) \mathcal{V}(\mathbf{\hat{r}}_{ij}) \right| \right> 
$$

(2.8)

Now expanding $e^{i \mathbf{k} \cdot \mathbf{\hat{r}}_{ij}} \approx 1 + i \mathbf{k} \cdot \mathbf{\hat{r}}_{ij}$ and similarly as $e^{i \mathbf{r}_{ij} \cdot \mathbf{\hat{r}}_{ij}}$, $(f_{k}^{\dagger})_{20}$ expression leads to form

$$
(f_{k}^{\dagger})_{20} = -\frac{1}{2a} \left< 2 \left| \frac{1}{m \omega_{20}^{2}} \sum_{i \neq j} i [\mathbf{k} \cdot \mathbf{\hat{r}}_{ij} \mathcal{V}(\mathbf{\hat{r}}_{ij})] \right| \right> 
$$

(2.9)

which is equivalent to a dipole approximation

$$
(f_{k}^{\dagger})_{20} = \frac{4}{a} \left< 2 \left| \left( \frac{1}{m \omega_{20}^{2}} \sum_{i \neq j} \mathcal{V}(\mathbf{\hat{r}}_{ij})^{2} \mathcal{V}(\mathbf{\hat{r}}_{ij}) \right) \right| \right> 
$$

(2.10)
Following the above expression for \( (\hat{\rho}_R^+)^{2\alpha} \), which is the same as obtained by Wong \(^3\), obviously this gives rise to the \( K_{ij} \) dependence of \( S_{P}(\vec{k},\omega) \) since it involves \( |C(\hat{\rho}_R^+)^{2\alpha}|^2 \). However, we adopt the technique based on the methods of quantum field theory to evaluate the matrix element \( (\hat{\rho}_R^+ \hat{\rho}_R^-)^{2\alpha} \) appearing in \( S_{P}(\vec{k},\omega) \).

As the state \( |2\rangle \) corresponds to double excitations is chosen to be of the form

\[
|2\rangle = \hat{\rho}_{p_1} \hat{\rho}_{p_2} |0\rangle
\]  

(2.11)

where

\[
\hat{\rho}_{p} = \sum_{P_3,6} c_{p_3,6}^+ c_{p_3,p_6}^+ \hat{c}_{P_3} \hat{c}_{P_6}^+ \hat{c}_{p_6} \hat{c}_{p_3}
\]  

(2.12)

In this \( c_{p_3,6}^+ c_{p_6} \) denotes the creation(annihilation) operator corresponding to a helium atom in liquid \( ^4\text{He} \), which being a Bose system, these operators obey the commutation relations.

\[
(\hat{\rho}_R^+ \hat{\rho}_R^-)^{2\alpha} = \langle 2 | \hat{\rho}_R^+ \hat{\rho}_R^- |0\rangle = \langle 0 | \hat{\rho}_R^+ \hat{\rho}_R^- |0\rangle
\]  

(2.13)

Writing the density fluctuation operator in terms of annihilation and creation operators and applying Wick's theorem to the product of boson operators, the matrix element \( (\hat{\rho}_R^+ \hat{\rho}_R^-)^{2\alpha} \) is evaluated. In this evaluation retaining the matrix element corresponding to
where the $\eta^i_{\mathbf{p}_i}$'s denote the distribution functions for the bosons. In this equation the terms inside the curly bracket within the delta function represent the energy corresponding to double excitation of liquid $^4$He. We now replace these terms by their respective averages. As a result, the terms of the type $\overline{\mathbf{q} \cdot \mathbf{q}}$ averages the zero, and hence give no contribution to the peak positions of

\[ S_{\Pi} (\mathbf{k}, \omega) \]. Now identifying the terms within the bracket \( \left\{ \frac{\epsilon_{\mathbf{p}_i}}{\mathbf{p}_i} \eta_{\mathbf{p}_i} \left[ 1 + \eta_{\mathbf{p}_1} \eta_{\mathbf{p}_2} \right] \right\} \)

with \( N^2 S(\mathbf{q}) S(\mathbf{q} + \mathbf{q}) \) where \( S(\mathbf{q}) \) denote the static structure function of the system, \( N \) is the average particle density in the system. Then we can write

\[ S_{\Pi} (\mathbf{k}, \omega) = \frac{4 N^2}{m^2 \omega} \sum_{\mathbf{q}} \frac{v^2(\mathbf{q}) (\mathbf{k} \cdot \mathbf{q})^2}{\omega^2} S(\mathbf{q}) S(\mathbf{q} + \mathbf{q}) \delta \left( \omega - \frac{\mathbf{k}^2}{2m} - \frac{\omega^2}{m^2} \right) \]

(2.15)

This identification have been made above in analogy with the Fermi system. This is in a sense is in keeping with the
work of Brandow\textsuperscript{50} and Lee\textsuperscript{51} who have established the similarity in treating both Bose and Fermi systems by bringing out an analogy between them. It can be trivially checked that by taking the definition of $S_{\Omega}(\omega)$ as
\[ S_{\Omega}(\omega) = \langle 0 \left| \hat{\phi}^+ \hat{\phi} \right| 0 \rangle \] and then applying Wick's theorem to the product of the boson operators averaged over the ground state of the system, one arrives at the same expression as shown above within the curly bracket.

We now make the assumption that any better decoupling procedure than the one mentioned above will lead to an exact $S_{\Omega}(\omega)$, than what we have written down. The very choice of writing $\{2\}$ in the way shown in Eq. (2.11) can only be justified provided one ignores correlations among the particles. We take care of the fluid correlations by replacing the unperturbed static structure functions appearing in (2.15) with the ones measured experimentally. From (2.15) it is apparent that the variation of $S_{\Omega}(\omega)$ with $\kappa$ is actually of order of $\kappa^2$. For small $\kappa$, we make a Taylor series expansion of $S_{\Omega}(\omega)$ to keep terms up to order $\kappa^2$. It is known that for large $q_\parallel$, that is for $q_\parallel > q_0$, a critical value $S_{\Omega}(\omega)$, go to unity. If one is in this large $q_\parallel$ region, from the argument of the delta function in (2.15) one immediately sees that this would automatically restrict one to large $\omega$ values given by $\omega = \frac{q_\parallel^2}{m} + \frac{\kappa^2}{m}$.
From the Taylor series expansion

$$S(\mathbf{q}, \omega^2) = S_0 + \sum_{n=1}^{\infty} \left( \frac{q^2}{\alpha_0^2} \right)^n \frac{\partial^n S(\mathbf{q}, \omega^2)}{\partial q^2}$$

Thus $S_\infty(\mathbf{q}, \omega)$ reduces to form

$$S_\infty(\mathbf{q}, \omega) = \frac{4\pi^2}{m^2 \omega_0^4} \sum_{k} \left[ \frac{\omega_0^2}{\omega} \left( \mathbf{q} \cdot \mathbf{q} \right)^2 \right]$$

$$\times \left\{ \frac{\omega_0^2}{\omega} + \frac{1}{2} \frac{k^2}{\alpha_0^2} - \frac{1}{2} \frac{\left( \mathbf{k} \cdot \mathbf{q} \right)^2}{\alpha_0^2} \frac{\partial^2 S(\mathbf{q}, \omega^2)}{\partial q^2} \right\}$$

$$\times \delta \left[ \omega - \frac{k^2}{\alpha_0^2} - \frac{q^2}{\alpha_0^2} \right]$$

(2.17)

The two pair contribution to dynamic structure factor in the region of large $\omega$ where $S(\mathbf{q}, \omega) \rightarrow 1$ reduces to the expression

$$S(\mathbf{q}, \omega) = \frac{N^2}{\pi^2} \frac{1}{m^2 \omega_0^4} \sqrt{\omega} \left[ \frac{4}{3} \frac{k^2}{\omega^{3/2}} - \frac{4}{3} \frac{k^2}{m \omega^{3/2}} \right]$$

(2.18)

where

$$V = \frac{u \kappa b}{m}$$

The region of low energy transfer would be determined by values $q$ less than $q_v$. In this region we choose
the form for \( s(q) \) as \(^4\)

\[
s(q) = \left[ \frac{2m c}{\omega} \right]^{-1} \left\{ |q^2| - 2 |q^2|^{3/2} \right\}
\]

(2.19)

where \( c = 237.5 \) meter/sec. is the isothermal sound velocity in liquid \(^4\)He in the superfluid phase and the parameters \( z = [4.5 \pm 0.2] \) \( A^2 \). For small \( \omega \)

the expression for \( S_\Pi(k^2, \omega) \) is given by

\[
S_\Pi(k^2, \omega) = \frac{N^2}{\pi^2} \frac{v^2}{m} k \mathcal{F}(k^2, \omega)
\]

(2.20)

where

\[
\mathcal{F}(k^2, \omega) = \frac{m k^2}{12 c^2} \left[ \frac{z^2}{\omega} \omega^{4/2} - \frac{2z}{m} \frac{1}{\omega^{1/2}} m^2 \frac{1}{\omega^{3/2}} \right]
\]

\[+ \frac{k_0^4}{80 c^2} \left[ \frac{z^2}{\omega \gamma_2} + \frac{6z}{m \omega^{3/2}} - \frac{7}{m^2 \omega^{3/2}} \right]
\]

(2.21)

**DISCUSSION:**

From equation (2.18) we notice that in the high energy region the dominant contribution from the multi excitations in liquid \(^4\)He is of order \( k^2 \omega^{-5/2} \) instead of \( k_0^4 \omega^{-7/2} \) as obtained by Family and Wong both. The frequency dependence of \( S_\Pi(k^2, \omega) \) is supposed to be different for different potentials. Extending our calculation to charged quantum systems we notice that for large \( \omega \) our \( S_\Pi(k^2, \omega) \) varies as \( \omega^{-9/2} \).
instead of \( \omega^{-1/2} \), a behaviour which has been reported by Family 36 and Wong 37. We have made a calculation of the intensity of the scattered neutrons for \( K = 0.6 \, \text{Å}^{-1} \) and \( K = 0.8 \, \text{Å}^{-1} \) in the high energy region using expression (2.18) starting from \( \omega = 70 \, K \) and going to lower values. For such momenta the intensity in the relatively low energy region is calculated from (2.20). On extrapolating the curves from both sides we notice that they meet at a point where \( \omega = 22.5^\circ \, K \) for \( K = 0.6 \, \text{Å}^{-1} \) and \( \omega = 22.1^\circ \, K \) for \( K = 0.8 \, \text{Å}^{-1} \). Both these numbers are very close to values of \( \omega \) at the positions of the second peaks that have been observed in the neutron scattering experiments 44,45 (which roughly comes out to be 20.07\(^\circ\)\,K and 24.5\(^\circ\)\,K respectively). Our results are shown along with the experimental data in Figs. (3) (4). From the graphs we find that our theoretical results agree very well with the experiment both in the high and low energy transfer region. It is interesting to notice that we have not used any adjustable parameters in our theory like those introduced by Wong 37 in order to fit with the experiment.

Thus we conclude that the second peak which is usually observed in the high energy region of the neutron scattering experiment from liquid \(^4\text{He}\) perhaps refers to the two phonon excitation mode, in conformity with
Fig. 3. Plot of Intensity of scattering Neutrons in arbitrary units versus energy loss in units of $k_0$. 

$k = 0.6 \text{ Å}^{-1}$ 

$T = 1.1 \text{ K}$
Fig. 4. Plot of intensity of scattering Neutrons in arbitrary units versus energy loss in units of K.

\[ k = 0.8 \, \text{Å}^{-1} \]
\[ T = 1.2 \, \text{K} \]
the interpretation given by Soda et al. Recently R. Shridhar et al. also have tried to explain the second peak in \( S(k^2, \omega) \) by looking at the two pair contribution. However their theory is phenomenological in the sense that the main result of this theory is derived by assuming a fitting formula for static structure function. From our expression for \( S(k^2, \omega) \) shown in eqn. (2.18) and (2.20), it is to be noticed that the contribution from the two phonon excitations varies as \( k^2 \). It is therefore obvious to think that there is a contribution to the \( f \)-sum rule to order \( k^2 \) coming from the two-phonon (pair) excitation of the system. This means that the one phonon excitation does not exhaust the \( f \)-sum rule to order \( k^2 \). We have discussed the implication of the dependence of \( S(k^2, \omega) \) on the various properties of system in section-II of this chapter.
SECTION-II

Contribution of \( S_n(\mathbf{k}, \omega) \) to various moments:

In the previous section our calculation of \( S_n(\mathbf{k}, \omega) \) indicates that the contribution from the two phonon excitation varies as \( k^4 \) rather than its \( k^4 \) dependence reported in earlier theories \(^{36,37}\). It is natural to think that the one phonon excitation alone cannot exhaust the \( f \)-sum rule \(^{48} \) to the order \( k^2 \). Thus we tried to make an estimation of the two phonon contribution to the \( f \)-sum rule for a set of \( k \) values. Using the expression for our \( S_n(\mathbf{k}, \omega) \) we have calculated, the static structure factor \( S_n(\mathbf{k}) \) of the system as a function of \( (\mathbf{k}^2) \), the values of \( S_n(\mathbf{k}) \) so obtained are fitted with a polynomial \(^{54} \) which is written down in power of \( \frac{k^2}{m_c} \) where \( c \) is the isothermal velocity of sound. Here we find that the coefficient of \( k^2 \) is finite instead of zero as given in earlier theories. Some further consequences of the presence of \( k^2 \) term are also being discussed in this paper.

To start with, we consider the frequency moments of \( S(\mathbf{k}, \omega) \) which are defined as

\[
\langle \omega \rangle_2 = \frac{1}{N} \int_{-\omega}^{+\omega} \omega^2 \, S(\mathbf{k}, \omega) \, d\omega
\]

where the index \( \ell \) refers to the various moments, \( N \) denotes the average particle density in the system, For
zero temperature the range of \( \omega \) integration in (2.22) is such that \( 0 < \omega < \infty \). Out of the various moments we confine ourselves to \( \epsilon = 0 \) and \( \epsilon = 1 \) in which case we have

\[
\langle \omega \rangle_0 = \frac{1}{\pi} \int_0^\infty \omega S(k^2, \omega) d\omega = S(k^2)
\]  

(2.23)

\[
\langle \omega \rangle_1 = \frac{1}{\pi} \int_0^\infty \omega S(k^2, \omega) d\omega = \frac{\hbar k^2}{2m}
\]  

(2.24)

where \( S(k^2) \), denotes the total static structure factor of the system in (2.23). Equation (2.24) which denotes the first moment is known as the \( \int \) sum rule. This is very important relation which follows as a direct consequence of particle conservation in the system. Higher moments are of limited interest to us since it is difficult to determine them experimentally.

The definition of \( S(k^2, \omega) \) which is given by (1.27) where \( \hat{f}_{R^2}^{(\alpha)} \) is the density fluctuation operator, the indices \( |0> \) and \( |n> \) respectively refer to the ground and excited states of many particle system which constitutes the liquid \(^4\text{He}\) in the present case as usual and \( \omega_{n0} = (E_n - E_0) \) is the excitation energy. Since in the region of high energy the two (pair) phonon excitation contribution to \( S(k^2, \omega) \) is expected to be large, in equation of (1.27) we
Using the confine ourselves to the case \( n = 2 \). Using the equation of motion for \( f_\mathbf{r}^+(t) \) and retaining the two phonon (pair) contribution term which is equivalent to evaluating the matrix element \( \langle f_\mathbf{k}^+ \rangle \mathbf{r} \). We have arrived at an expression for \( S_\Pi(\mathbf{r}, \omega) \), Eqs. (2.18) and (2.20) in the last chapter. From the eqns. (2.18) and (2.20) it is apparent that the variation of \( S_\Pi(\mathbf{r}, \omega) \) with \( \mathbf{k} \) is order of \( \mathbf{k}^2 \). Thus the contribution to \( f \)-sum rule can be calculated.

To evaluate \( S_\Pi(\mathbf{r}, \omega) \) we can write

\[
S_\Pi(\mathbf{r}, \omega) = \frac{4}{n} \int_0^\infty S_\Pi(\mathbf{r}, \omega) \, d\omega
\]  

(2.25)

In this evaluation of two pair/phonon contribution to static structure function we have to choose proper limits of \( \omega \). The lower limit of \( \omega \) is determined from the fact that \( S_\Pi(\mathbf{r}, \omega) \) is zero below such a value of \( \omega \) for any fixed \( \mathbf{k} \). This lower limit was denoted by \( \omega_1 \). Thus as regards the estimation of \( S_\Pi(\mathbf{r}, \omega) \) is concerned, the integration over \( \omega \) is broken up as follows

\[
\int_0^\infty \omega \, d\omega = \int_{\omega_1}^{\omega_2} \omega \, d\omega + \int_{\omega_2}^{\infty} \omega \, d\omega
\]  

(2.26)

where \( \omega_2 \) corresponds to the value of \( \omega \) at which the high and low energy curves in the \( S_\Pi(\mathbf{r}, \omega) \) plot in Fig. (3,4) meet. This should in principle be given by the two phonon excitation frequency. The \( S_\Pi(\mathbf{r}, \omega) \) values for \( \mathbf{k} = 0.3, 0.6, 0.9 \) and \( 1.0 \mathbf{A}^2 \) have
<table>
<thead>
<tr>
<th>$k (\text{A}^{-1})$</th>
<th>$S_{II}(k)$</th>
<th>Up to $k^2$</th>
<th>Upto $k^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.00425</td>
<td>0.00429</td>
<td></td>
</tr>
<tr>
<td>0.6</td>
<td>0.01736</td>
<td>0.017572</td>
<td></td>
</tr>
<tr>
<td>0.8</td>
<td>0.0311</td>
<td>0.0314785</td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td>0.0554</td>
<td>0.048</td>
<td></td>
</tr>
</tbody>
</table>
been calculated and are shown in Table 1. These \( S(\kappa^2) \) values have been tried to be fitted with a polynomial of the form:

\[
S(\kappa^2) = S_I(\kappa^2) + S_{II}(\kappa^2) = \frac{k \kappa}{2mc} \left[ 1 + Z_2 \frac{k \kappa}{mc} + Z_3 \left( \frac{k \kappa}{mc} \right)^2 + Z_4 \left( \frac{k \kappa}{mc} \right)^3 + \ldots \right] (2.27)
\]

\( c \) being the isothermal sound velocity in superfluid helium. The above form of \( S(\kappa^2) \) is written using the expansion formula for the structure function corresponding to the excitation of single-phonon, and that for \( S_{II}(\kappa^2) \) which has been shown to vary as \( \kappa^2 \). Comparing the calculated values for \( S_{II}(\kappa^2) \) with those obtained from above Eqn. (2.27), it is found that the expansion coefficient \( Z_2 \) associated with the factor \( \frac{1}{2} \left( \frac{k \kappa}{mc} \right)^2 \) assumes a value of \( \approx 0.21 \). This value of \( Z_2 \) has been seen to remain the same for all four values of \( \kappa \) for which \( S_{II}(\kappa^2) \) has been evaluated. This coefficient \( Z_2 \) was obtained to be zero in many earlier theories, whereas the present theory gives a value of 0.21.

The coefficient of the terms \( \frac{1}{2} \left( \frac{k \kappa}{mc} \right)^3 \) and \( \frac{1}{2} \left( \frac{k \kappa}{mc} \right)^4 \) in equation (2.27) which have been denoted by \( Z_3 \) and \( Z_4 \) respectively have the values \( \approx 3.5 \) and \( \approx 5.8 \) when expressed in dimensionless units. On comparing estimated \( Z_2 \) with the value of \( Z_3 \) and \( Z_4 \).
it is found that $Z_\omega$ is actually very small. The comparison between coefficient of $k^2$ to that of $k^4$ has been done for other system as charged Bose gas. The (coefficients of $k^4$/the coefficient of $k^2$) term for charged Bose gas is 2.82 as against the value of 27.6 obtained by the present calculation for the neutral Bose gas. It looks as if the coefficient of $k^4$ is greater than coefficient $k^2$ in both charged as well as neutral Bose system. The very estimation of $Z_\omega$ made above is a direct consequence of the fact that $S_\Pi (k^2)$ varies as $k^2$. Since such variation of $S_\Pi (k^2)$ with $k$ has been missed by several workers one might think it to be an outcome of the approximation that has led us to write $S_\Pi (k^2)$ in the form,

$$S_\Pi (k^2) = \int_{-\omega}^{+\omega} \frac{4 N^2}{m^2 \omega^4} d\omega \sum \frac{V^2 (q^2, (k^2, q^2)^2}{q^2}$$

$$S(q^2, S(q^2 + k^2) S(\omega - \frac{q^2}{m} - \frac{k^2}{2m})$$

Another attempt has been made to derive $S_\Pi (k^2)$ starting from an altogether different consideration. The new derivation is based on the knowledge of the two phonon propagator which is analogous to the expression for the two plasmon propagator obtained by Deo and Tripathy sometime back. In the present calculation, the four
particle density response function is used to evaluate
the two-phonon propagator for the neutral Bose gas.

The four particle density function is defined as

$$F_0(\mathbf{q}, \omega) = \frac{i}{8\pi^2} \int \frac{d^3 \mathbf{p}}{n_2} \frac{1}{R_2(\mathbf{p}^2, \omega + \epsilon)}$$

where $\mathbf{p}$ denotes the density operator in the Heisenberg
representation, $\gamma$ is the exact ground state of many
boson system. The perturbative expansion for $F_0$ is
written down using the methods of quantum field theory of
many particle system [56]. According to this the
propagator for two pair/phonon excitation can be written
as

$$F_0(\mathbf{q}, \omega) = \frac{i}{(2\pi)^4} \left( \int \frac{d^3 \mathbf{p}}{n_2} \frac{1}{R_2(\mathbf{p}^2 + \mathbf{q}^2, \omega + \epsilon)} \right)$$

where [57]

$$R_2(\mathbf{p}, \epsilon) = - \frac{i}{\epsilon} \int_{-\infty}^{\omega} d\omega' \epsilon \int_0^{\omega'} \frac{d\omega''}{\omega''} \left<\mathbf{0} | T \mathbf{p} \mathbf{p}^{(0)} | \mathbf{0}\right>$$

In the above expansion only free propagator of two
pair/phonon is written down. The term containing inter-
action of two phonon will give higher order correction.

$R_2(\mathbf{p}, \epsilon)$ consists of the spectrum due to the
excitation of two pairs and two phonon, where the phonon
refers to some coherent mode of propagator of the particles in the system. These are more familiarly known as the zero sound in a many particle system. Retaining the phonon part of the spectrum in \( R_2(\vec{p}, \epsilon) \) it can be expressed as

\[
R_2(\vec{p}, \epsilon) = \lim_{\eta \to 0^+} \frac{-2 \omega^2(\vec{p})}{2 \nu(\vec{p}) \{ (\omega^2(\vec{p}) - \epsilon^2 \eta) \}}
\]

where \( \omega(\vec{p}) = C(\vec{p}) \) and \( |\vec{p}| \) represents the momentum transfer. \( C \) is the isothermal sound velocity and \( \nu(\vec{p}) \) is some critical wave vector up to which the one phonon excitation exists as a well defined mode and \( \nu(\vec{p}) \) is the Fourier transform of the interparticle potential.

In the above expression for \( R_2(\vec{p}, \epsilon) \) if \( \nu(\vec{p}) \) is written as \( \frac{4 \pi e^2}{\vec{p}^2} \) i.e. the Fourier transform of the Coulomb potential between a pair of electron then \( R_2 \) will represent the one plasmon propagator in a many electron system. In case of \( ^4He \) \( \nu(\vec{p}) \) can be taken as delta function type thus \( \nu(\vec{p}) \) is constant with respect to momentum variable. Thus \( F_0 \) is written as

\[
F_0(\vec{r}, \omega) = \frac{1}{(2\pi)^3} \frac{1}{N^2} \int d\vec{P} \frac{\omega(\vec{P}) \omega(\vec{P} + \vec{r})}{\nu(\vec{P}) \nu(\vec{P} + \vec{r})} \left[ \frac{1}{\omega(\vec{P}) - \omega(\vec{P} + \vec{r}) + i\eta} - \frac{1}{\omega(\vec{P}) + \omega(\vec{P} + \vec{r}) - i\eta} \right]
\]

Then dynamic structure factor \( S_\Omega(\vec{r}, \omega) \) is defined as

\[
S_\Omega(\vec{r}, \omega) = -\frac{1}{\pi} \text{Im} \left. F_0(\vec{r}, \omega) \right|_{\nu \neq 0}
\]
where $N$ denotes average particle density in the system. Using expression for $F^0(k^3, \omega)$ in expression of $S^0_{\Pi}(k^3, \omega)$, $S^0_{\Pi}(k^3, \omega)$ reduces to form

$$S^0_{\Pi}(k^3, \omega) = \frac{1}{(2\pi)^3} \frac{1}{N^2} \int \frac{d^3p}{4 \sqrt{v^2}} \frac{\omega(\vec{p}) \omega(\vec{p} + \vec{k})}{v^3 \omega(\vec{p} + \vec{k})} \delta \left( \omega - \omega(\vec{p}) - \omega(\vec{p} + \vec{k}) \right) \quad (2.35)$$

Thus definition of $S^0_{\Pi}(k^3, \omega)$ used above is in keeping with the well known definition of the dynamic structure factor for one pair (phonon) excitations. Here $\delta(\omega)$ being a delta function type of potential the Fourier transform of the potential is given by

$$V(\vec{p}) = \frac{4\pi b}{3} \quad (2.36)$$

where $b$ is scattering length and $m$ is the mass of superfluid $^4$He atom. Following the equation (2.25) the expression for static structure factor can be obtained using the relation

$$S^0_{\Pi}(k^3) = \frac{1}{N} \int S^0_{\Pi}(k^3, \omega) d\omega$$

$$= \frac{1}{N^3} \frac{1}{(2\pi)^3} \int \frac{d^3p}{4 \sqrt{v^2}} \frac{\omega(\vec{p}) \omega(\vec{p} + \vec{k})}{v^3 \omega(\vec{p} + \vec{k})} \int d\omega \delta \left( \omega - \omega(\vec{p}) - \omega(\vec{p} + \vec{k}) \right) \quad (2.37)$$

$$S^0_{\Pi}(k^3) = \frac{1}{N^3} \frac{1}{(2\pi)^3} \frac{1}{4 \sqrt{v^2}} \int d^3p \omega(\vec{p}) \omega(\vec{p} + \vec{k}) \quad (2.38)$$
To evaluate the above integral the linear part of the phonon spectrum \( \omega(p) = C \cdot p \) is considered. For small \( \mathbf{k} \) values \( k^2 \)-dependent term in \( S_\mathbf{u}(K^2) \), is obtained which is given by \( C^2 \mathbf{k}^2 / (4 \pi^2 M^2 v^2) \). Thus in this type of evaluation of static structure factor, for the two phonon excitation following the definition of two phonon propagator also leads us to \( k^2 \)-dependent term. This result is in contrast with the earlier theories.

Thus \( S_\mathbf{u}(K^2, \omega) \) varies as \( k^2 \) and it may contribute to \( f \)-sum rule to order \( k^2 \). To estimate the contribution it can be written as

\[
\left( \frac{\mathbf{k} \cdot \mathbf{k}^2}{2 m^2} \right)^{-1} \frac{1}{N} \int_0^{\infty} \omega \, s_\mathbf{u}(K^2, \omega) \, d\omega = 1
\]

(2.39)

where

\[
H_+ + H_- = 1
\]

(2.40)

Following the expression for \( S_\mathbf{u}(K^2, \omega) \) in eqn. (2.18, 2.20) in the high and low energy region, we estimate the value of the integral on the left hand side of eqn. (2.39) for the set of \( k \)-values used for evaluating \( Z_2 \). Those are shown in table-II. From this table it is noticed that the value of the above integral
### Table 2

$H_{II}$ for different $k$ values

<table>
<thead>
<tr>
<th>$k (\text{R}^{-1})$</th>
<th>$H_{II}$ up to $k^2$</th>
<th>$H_{II}$ up to $k^4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3</td>
<td>0.44548</td>
<td>0.44406</td>
</tr>
<tr>
<td>0.6</td>
<td>0.44918</td>
<td>0.439</td>
</tr>
<tr>
<td>0.8</td>
<td>0.45054</td>
<td>0.43082</td>
</tr>
<tr>
<td>1.0</td>
<td>0.462966</td>
<td>0.405152</td>
</tr>
</tbody>
</table>
which is denoted by \( \beta \) is less than \( n \) for \( k < 1.01 \)
where \( n \) is obtained replacing \( S_{\Pi}(\vec{K}, \omega) \) by
\( S_{\Pi}(\vec{K}, \omega) \) in eqn. (2.40). This result is in contrast
to what has been done by Cowley, Woods. Since the
value of \( n \) is found to be decreasing with increasing \( k \)
this indicates that beyond certain \( k \), the contribution
to \( S_{\Pi} \) would be vanishingly small. This is manifested
in the fact that the height of the second peak observed
in the neutron scattering experiment almost disappear
at larger \( k \) values. If this be the case \( S_{\Pi} \) would
dominate for large \( k \) values which would finally
approach unity beyond certain critical values of \( k \).
This is what observed for a quantum liquid like the
system of electron gas at \( T = 0 \). Because of this
one does not see any reason why the system of super-
fluid \(^4\text{He} \) would behave differently from an electron
liquid at \( T = 0 \).

To summarise, the one phonon excitation in
superfluid \(^4\text{He} \) system do not alone exhaust \( \sum \)-sum rule
to the order \( k^2 \). \( S_{\Pi}(\vec{K}, \omega) \) evaluated by this present
calculation seems to contribute to the \( j \)-sum rule. The
coefficient of \( k^2 \) of the static structure factor is
found to be finite instead of being zero as known from
earlier theories.
AN EXPLANATION OF THE STRUCTURE IN THE DYNAMIC STRUCTURE FACTOR OF AN ELECTRON LIQUID
SECTION-I

Introduction

In this chapter we essentially try to explain the structure that has been recently observed in the intensity of the inelastically scattered x-rays and electrons from metals. As we have seen the intensity of these x-rays and electrons is directly related to the dynamic structure factor $S(r,\omega)$ of the system. If one carefully looks at the structure in $S(r,\omega)$ of various metals, and compares it with that of the observed in superfluid $^4$He, one can notice that there is a great similarity in the behaviour of $S(r,\omega)$ versus $\omega$ for both the systems. As we know by now the systems constitute two different class of quantum fluids in the limit of zero temperature. One is a Fermi liquid and the other one is a Bose liquid. The type of Bose liquid we come across in liquid $^4$He below $T = 2.17$ K is of the superfluid family. Before we go to explain theoretically the observed structure in $S(r,\omega)$ of metals, let us discuss briefly about its occurrence and the various theoretical explanations that have been put forth to explain this physically prior to us. The inelastic scattering experiments from metals, using x-rays as the incident beam is mainly due to Platzman and Eisenberger and that using the electron beam is due to Gibbons et al. P. Zacharias and Batson et al. All these experiments indicate that there is a double peak structure
in the plot of $\delta(\mathbf{q}, \omega)$ versus $\omega$ for several metals for like Li, Be, Al, Na and even for graphite in the momentum transfer region $K_c < K < 2K_F$, where $K_c$ is the critical wave vector up to which the plasmons exist as well defined collective modes of the system of electron gas, and $K_F$ is the Fermi wave vector of the system. Since the spectrum of $\delta(\mathbf{q}, \omega)$ of different metallic systems mentioned above looks very similar, one concludes that the structure in $\delta(\mathbf{q}, \omega)$ should be dependent on some general property of the solid state electron gas rather than on band structures of these systems. This is because the band structure of these varieties of systems are quite different from each other since the plasmons exist up to $K_c$ for $K < K_c$, the spectrum of $\delta(\mathbf{q}, \omega)$ is expected to be dominated by the plasmon contribution and for higher values of momentum, that is for $K = 2K_F$, it is to be purely given by the particle-hole excitation spectrum. Therefore to account for the structure in the intermediate momentum transfer region $K_c < K < 2K_F$, it was argued that the spectrum in this region perhaps is constituted of two parts: one broad component which corresponds to the particle-hole excitations and other a relatively sharp component which has been interpreted as due continuation of the plasmon modes into the momentum transfer region beyond $K_c^{RPA}$ without caring for the existence of the plasmon modes.
to region beyond \( k_c \) there have been attempts to calculate \( S(\mathbf{r}, \omega) \) using the dielectric function of the random phase approximation (RPA) and that of Vashishta and Singwi\(^{73} \) (hereafter to be called as VS-theory) which goes beyond the RPA. As we know the \( S(\mathbf{r}, \omega) \) is related to the dielectric function of the system through the fluctuation dissipation theorem which is stated as follows

\[
S(\mathbf{r}, \omega) = \frac{k^2}{4\pi \varepsilon^2} \text{Im} \left[ \frac{1}{\varepsilon(\mathbf{r}, \omega)} \right]
\]  

(3.1)

Evaluation of \( S(\mathbf{r}, \omega) \) done using the RPA dielectric function and the one due to Vashishta and Singwi do not reveal any structure in \( S(\mathbf{r}, \omega) \). In a later work by Mukhopadhyay et al\(^{68} \), which makes use of a modified form of the VS-dielectric function incorporating lifetime effects in the local field factor, an evaluation of \( S(\mathbf{r}, \omega) \) is done as a function of \( \omega \) for several values of \( k > k_c^{RPA} \). In this case there seems to have appeared some structure in \( S(\mathbf{r}, \omega) \). The results of this work has been afterwards verified by Rao et al\(^{76} \) by means of a rigorous treatment of lifetime effects in the free electron-hole propagator. Their calculation show without any doubt that there is no such structure in \( S(\mathbf{r}, \omega) \) in the region \( k > k_c^{RPA} \) for any of the systems mentioned above. This obviously shows that the structure in \( S(\mathbf{r}, \omega) \) cannot be accounted for due to assignments...
of finite life times to particles and holes. Another calculation of \( s(\omega) \) by Raedt and Raedt 70 which is based on the derivation of a dielectric function following Mori's memory function formalism seemed to have further indicated the presence of structure in \( s(\omega) \), but again there are several objections against this theory, as this deals with several adjustable parameters in order to reproduce the structure. Some of these parameters are even found to be dependent on momenta. As such they vary drastically in going to the limit of large wave vectors. Along with these deficiencies, the dielectric function used by Raedt and Raedt, for the evaluation of \( s(\omega) \) also violates the compressibility sum rule, and further more it does not go to unity in the limit of large, \( \omega \), a well established result in the asymptotic limit. From all these considerations, the theory by Raedt and Raedt cannot be understood from first principles. It is also not clear from their theory, what effects are actually responsible for giving rise to the structure. The calculation by Barnea 72 which enables him to consider the process involving the decay of a plasmon into an electron hole pair plus a plasmon in addition to the usual RPA single pair decay, reproduces a structure in \( s(\omega) \) similar to the one reported by the experiment. This theory makes use of a ansatz to evaluate the matrix elements associated with the decay of the plasmon into the above two processes.
The basic question that the plasmons actually exist beyond the $K_c$ remains unanswered in this theory. Besides, this theory leads to the unphysical feature of having a negative value of $\Sigma(k,\omega)$ for higher frequencies. Therefore, what it appears from the varieties of discussions presented above is that the explanation of the structure in $\Sigma(k,\omega)$ is in a state of utter confusion. A much later calculation of $\Sigma(k,\omega)$ by Awa et al shows that it is possible to reproduce the two peak structure by incorporating damping effects of one electron states originating from virtual plasmon emission under the influence of short range correlations at metallic densities. The results of this calculation go against the earlier criticism by Rao et al that the structure in $\Sigma(k,\omega)$ cannot be due to lifetime effects of the particle hole pairs. Besides it involves such a cumbersome numerical computation that one cannot easily see what is precisely responsible for the structure. Furthermore there are several approximations within the theory which needs to be justified. A similar calculation by Green et al to explain the structure is worth mentioning. The result of this work shows that the two peak structure in $\Sigma(k,\omega)$ is generated by dynamic correlation effect between pairs of electrons but not due to collective effects. In view of this calculation by Awa et al
looks doubtful. Therefore, if one has to believe in the explanation that the structure in $\mathcal{S}(R^2, \omega)$ in the region $k_c < k < 2k_F$ is due to the superposition of the plasmon and quasiparticle excitation spectrum, it is very much necessary to show that the plasmons actually exist up to wave vectors beyond $k_c^{\text{RPA}}$. Where as in the RPA, the plasmon is known to terminate sharply at $k_c$ whose value is given by $\approx 0.47 \gamma_5 \frac{\sqrt{2}}{\epsilon} k_F$. Keeping this in view theoretical studies have been made by Pal et al. and by Tripathy and Pal to see whether the plasmons exist beyond $k_c^{\text{RPA}}$. In these works, the frequency of the plasmon mode has been calculated taking into consideration the contributions from beyond the RPA. In one of these papers, the one plasmon propagator was evaluated using the perturbative methods of the quantum field theory of many-body systems by treating the electron-plasmon interacting term as perturbation. The poles of this propagator are analyzed to determine the plasmon frequency as a function of the momentum transfer to the system. In the other approach, a microscopic dielectric function of an interacting electron gas with a neutralizing uniform positive background was obtained by taking into account solely the contributions due to the exchange of virtual plasmons along the self-energy correction diagrams of
a particular kind to the free electron-hole propagator. The zeroes of this dielectric function are investigated to find the plasmon dispersion. In both the approaches, an evaluation of the plasmon frequency in the long wavelength limit (that is at $k = 0$) is made. Such calculations indicate that there is a frequency shift to the classical plasma frequency $\omega_{pl}$ and this is seen for several metals. The recent experimental data obtained by Eisenberger et al., Zacharias and Gibbons et al. also indicate such a frequency shift to the classical plasma frequency and its value in most of the metals is of the order $\approx 0.9 \omega_{pl}$. This is reported to be an universal value for most of the metallic systems. To reproduce the actual experimental value for the frequency shift, Pal et al. and Tripathy and Pal use $k_c'$ as an adjustable parameter in their theories. By doing so they arrive at a new value of $k_c$ which is much beyond $k_c^\text{RPA}$ ($k_c^\text{RPA} = 0.27 \tau_5^{1/2} k_F$) for any system. However, this value of $k_c$ which they arrive at, does not go up to $2k_F$ at which the structure in $\Sigma(k, \omega)$ is being observed.

Having shown the extension of the plasmon mode to region beyond $k_c^\text{RPA}$, Tripathy and Pal have calculated $\Sigma(k, \omega)$ versus $\omega$ by taking into account both the plasmon and quasiparticle excitation contributions to $\Sigma(k, \omega)$. This calculation does not reveal any kind of structure in $\Sigma(k, \omega)$ at the values $k_c < k < 2k_F$. 

82"
With this it is unequivocally proved that the observed structure certainly cannot be due to the superposition of the plasmon and quasiparticle excitation spectrum.

Recently, a theory for a strongly interacting electron liquid at metallic densities has been developed by Kenichi Utsumi and Setsu Ichimaru (hereafter referred as UI) in which the dielectric response function obtained by the authors accounts for strong coupling effects through the introduction of three characteristic functions such as (i) the localised correction factor $q(R)$, (ii) relaxation time $\tau(R)$ in the long time domain and (iii) the relaxation frequency in the short time domain denoted by $\Omega(R)$. The frequency $\Omega(R)$ is determined in such a way that the dielectric function satisfies the third frequency moment sum rule. The relaxation time $\tau(R)$ refers to the collision time due to Coulomb scattering between pair of electrons in the many electron system. Each of the above three functions in the UI theory is being expressed as functional of the static structure factor. The UI formulation has certain interesting features like the appearance of a peak in the static structure factor $S(R)$ and the local field factor $g(R)$ at $k \approx 2k_F$, similar to the one reported by Tripathy, Mandal and Rao sometime back, a calculation based on the dielectric function derived by Tripathy and
Mandal 85. The most interesting result of the UI-dielectric function is that it reproduces a good pair correlation function $g(r)$ at $|\tau'| = 0$ in the range of metallic density. In spite of all these nice features, the UI-theory is not capable of reproducing the double peak structure in $\Sigma(\mathbf{q}, \omega)$ as reported by the inelastic scattering experiments 53-66 from metals.

We have taken up a quite different view to explain the structure by assuming that this is due to superposition of one and multipair excitation spectrum. The reason for believing like this arises because of our success in explaining the double peak structure in the dynamic structure $\Sigma(\mathbf{q}, \omega)$ spectrum of liquid $^4$He reported by Cowley and Woods. Details of this has been mentioned in the chapter-II of this thesis. We think that the mechanism for giving rise to the structure in $\Sigma(\mathbf{q}, \omega)$ for the electron liquid is same as that of liquid $^4$He which is well known Bose liquid. In other words, in this chapter we give an estimation of the dynamic structure corresponding to two pair excitation in an electron liquid and using this we try to explain the double peak structure. The details of the calculation is given in the next section of this chapter.
SECTION-II

THEORY

We start with the familiar expression for the intensity of the scattered beam which is written as

\[ I(\mathbf{k}, \omega) = \left( \frac{\partial S}{\partial \omega} \right)_0 S(\mathbf{k}, \omega) \]  

(3.2)

where

\[ S(\mathbf{k}, \omega) = S_1(\mathbf{k}, \omega) + S_\Pi(\mathbf{k}, \omega) \]  

(3.3)

\( S_1(\mathbf{k}, \omega) \) being the contribution from one pair excitation to the dynamic structure function and \( S_\Pi(\mathbf{k}, \omega) \) the contribution due to two pair excitations. Following the definition of the dynamic structure factor of a many particle electron gas as given by (1.27), we have restricted ourselves to consider only two pair contribution, i.e., to calculate the contribution from \( n = 2 \) state. Here also \( \mathbf{27} \) states represent ground state of the electron gas system. Thus to calculate the two pair contribution we have followed the same method for both superfluid \(^4\text{He}\) as well as electron gas. The proper expression for Hamiltonian is chosen as (2.2) and the equation of motion for appropriate density matrix is obtained as

\[ \dot{\tilde{p}}_k^\dagger(t) = -\sum_{i=4}^N \left( -\frac{\mathbf{K} \cdot \tilde{p}_i}{m} + \frac{\mathbf{K}^2}{2m} \right)^2 \tilde{e}^{i\mathbf{K} \cdot \overline{\mathbf{r}}_i(t)} \]

\[ + \sum_{\tilde{q}} \mathcal{V}(\tilde{q}) \frac{\mathbf{K} \cdot \overline{\mathbf{q}}}{m} \tilde{p}_{\overline{\mathbf{K}} - \overline{\mathbf{q}}}(t) \overline{\tilde{p}}_{\overline{\mathbf{q}}}(t) \]  

(3.4)
with
\[
\begin{align*}
(\hat{p}_{\mathbf{R}_0}^+(t))_{n_0} &= \langle \eta | \hat{p}_{\mathbf{R}_0}^+(t) | 0 \rangle = e^{-i \omega_{n_0} t} (\hat{p}_k^+)_{n_0} \tag{3.5}
\end{align*}
\]
and
\[
\hat{p}_{\mathbf{R}_0}^+(t) = \sum_{c = 1}^{N} e^{i \mathbf{R}_0 \mathbf{r}_c(t)} \tag{3.6}
\]
where \( V(\mathbf{q}) = \frac{4 \pi \varepsilon^2}{q^2} \) denotes the Fourier transform of Coulomb potential between a pair of electrons in the many electron system. As similar to the details done in chapter II separating time dependence of density fluctuation operator the matrix element for \((\hat{p}_{\mathbf{R}_0}^+)_{n_0}\) is obtained as follows:
\[
(\hat{p}_{\mathbf{R}_0}^+)_{n_0} = \langle 2 | \hat{p}_{\mathbf{R}_0}^+ | 0 \rangle = -\sum_{\mathbf{q}} \omega_{20}^{-1} (\frac{\mathbf{R}_0 \mathbf{q}}{m}) V(\mathbf{q}) \langle 2 | \hat{p}_{-\mathbf{R}_0 \mathbf{q}} | 0 \rangle \tag{3.7}
\]
To evaluate the matrix element in r.h.s. of the above equation we adopt a similar procedure as done for \(^4\text{He}\) which is a Bose gas, the only difference lies in the fact that the creation and the annihilation operators here belong to the Fermi class of particles and hence they obey anticommutation relations. The second quantised version of \(\hat{p}_{\mathbf{R}_0}\) is written as
\[
\hat{p}_{\mathbf{R}_0} = \sum_{\mathbf{p}, \sigma \neq \mathbf{p}_0, \sigma} \hat{c}_{\mathbf{p}, \sigma}^\dagger \hat{c}_{\mathbf{p} + \mathbf{R}_0, \sigma} \tag{3.8}
\]
and \(\hat{c}_{\mathbf{p}, \sigma}^\dagger \hat{c}_{\mathbf{p}, \sigma}\) denotes the creation and annihilation
operators for electron gas
\[ [C_p, C_{p'}^+] = \delta_{p, p'} \]  \hspace{1cm} (3.9)

By writing the state \(|2\rangle\) as
\[ |2\rangle = \prod_{\vec{p}} \frac{1}{\sqrt{\omega_{\vec{p}}} \omega^{\frac{1}{2}}} \]  \hspace{1cm} (1.10)
and using equation (3.9) and applying Wick's theorem to product of Fermi operators we write two pair contribution to dynamic structure factor \(S_{\Pi}(\vec{q}, \omega)\) as follows
\[
S_{\Pi}(\vec{q}, \omega) = \sum_{\vec{p}, \vec{p}', \vec{q}_1} \frac{1}{\omega_{\vec{q}_1} \omega^{\frac{1}{2}}} \chi^2(\omega_{\vec{q}_1}) \chi^2(\omega_{\vec{q}_1}) \chi^2(\omega_{\vec{q}_1}) \chi^2(\omega_{\vec{q}_1})
\]
\[
\times \left[ -\gamma \left( 1 - n^F_{\vec{p}} + \omega_{\vec{q}_1} - \omega_{\vec{q}_1} \right) n^F_{\vec{p}} (1 - n^F_{\vec{q}_1} + \omega_{\vec{q}_1} - \omega_{\vec{q}_1}) \right]
\]
\[
\delta \left[ \omega - \left( \frac{\vec{q}_1^2}{m} + \frac{k^2}{m} + \frac{\vec{q}_2^2}{m} + \frac{\vec{q}_1^2}{m} + \frac{\vec{q}_2^2}{m} \right) \right]
\]  \hspace{1cm} (3.11)

where \(n^F\) denotes the distribution function for the Fermions. The \(n^F\)'s are such that at zero temperature
\[
n^F = \begin{cases} 1 & \text{for } |\vec{p}| < k_F \\ 0 & \text{otherwise} \end{cases}
\]  \hspace{1cm} (3.12)

From the equation (3.11) it is obvious that in this equation there are two electrons having momenta \(|\vec{p}_1|\) and \(|\vec{p}_2|\) less than \(k_F\) the Fermi momentum which are excited to states having momenta \(|\vec{p}_1 + \vec{q}_1 + \vec{q}_2|\) and \(|\vec{p}_2 + \vec{q}_1|\) which are greater than \(k_F\). This is the matrix element corresponding to the direct process.

Evaluation of the integral involved in the equation (3.11) is certainly very complicated. We approximate the terms
within the argument of the delta function by their angular average values. As pointed out by Woods and Cowley 48 the terms of type \( q^2 \cdot \vec{P} \) give no contribution to the peak position but are responsible for the width about \( \frac{q^2}{2m} \). To compensate for the use of such an approximation we introduce a parameter \( \alpha \) into our theory. This is done by writing \( \frac{\alpha k^2}{2m} \) instead of \( \frac{k^2}{2m} \) in the argument of the delta function. As it looks the parameter \( \alpha \) has been used to take care of the \( k \) dependence of the terms those are averaged out to zeros. The value of this parameter is fixed from the best fit within the experimental data. With these approximations the above expression for the \( S_{\Pi}(k^2, \omega) \) is simplified as follows:

\[
S_{\Pi}(\vec{R}, \omega) = \frac{4\pi^2}{m^2 \omega^4} \sum_{q^2} v^2 \delta^2(q^2) (\vec{R} \cdot \vec{q})^2
\]

\[
S_{\Pi}(\vec{R} + \vec{q}) \delta (\omega - \frac{q^2}{m} - \frac{\alpha k^2}{2m})
\]

where \( S(q^2) \) denotes the static structure factor of the system such that

\[
\sum_{\vec{p}^2} \frac{s_{\Pi}(\vec{p})}{\vec{p}^2} (1 - \frac{s_{\Pi}(\vec{p} + \vec{q})}{s_{\Pi}(\vec{q})}) = N s_{\Pi}(\vec{q})
\]

In the absence of any analytical form of \( s_{\Pi}(\vec{q}) \) either in the RPA and beyond we shall be using its Hartree Fock value 12 for evaluating the integral for \( S_{\Pi}(k^2, \omega) \). An estimation of \( S_{\Pi}(k^2, \omega) \) as a function of \( \omega \) is done numerically for systems like Li, Be, Al metals and graphite corresponding to several values of wave vectors.
Fig. 5. Plot of Intensity of $S(R, \omega)$ versus $\omega/E_F$. The — represents our theory and —— represents experimental result.
Fig. 6. Plot of Intensity of $\chi_{k}^{-1}(\omega)$ versus $\omega/E_F$. The solid line represents our theory, and the dashed line represents the experimental result.