

STUDY OF THE DYNAMICAL BEHAVIOUR OF CERTAIN MANYBODY SYSTEMS



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TO



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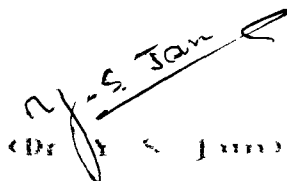
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(Dr. Y. S. Jan)
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SYNOPSIS

The dynamical behaviour of manybody systems has been a subject of research for a long period. It provides a very good understanding of inter- and intra-particle interactions, which serve as the starting base for developing the microscopic model for the behaviour of a system and testing ground for different laws of nature. Over the past few decades, there has been a growing interest in the study of the dynamical behaviour of molecules, liquids and solids.

Liquid Helium is an interesting manybody system which does not solidify even at $T \approx 0K$. At $T_\lambda = 2.17K$ it undergoes a second-order phase transition and transforms from its normal phase (He-I) to its superfluid phase (He-II). Some of the important properties of He-II are: (i) Superfluidity, (ii) high thermal conductivity, (iii) negative volume expansion, (iv) singularity at $T = T_\lambda$ in the specific heat and related properties, (v) capacity to sustain the propagation of temperature waves, etc. Several efforts have been made to develop the theory of He-II [1] but the real microscopic picture of its unique behaviour has not emerged for a long time. The physics of He-II has, therefore, been understood in terms of two fluid phenomenology developed by

Landau [2]. Attempts have been made to strengthen this model by microscopic calculations of $k=0$ condensate [3] assuming that such condensate is related to the superfluid density. However, the existence of $k=0$ condensate has not been confirmed experimentally even after repeated efforts. In addition, the fact that 1-D and 2-D systems of He-II exhibit superfluid behaviour while the existence of $k=0$ condensate in these systems, is theoretically ruled out, indicates that $k=0$ condensation is not essential for superfluid behaviour.

He-II has always been presumed to have a random distribution of its atoms in normal and superfluid phase, while the fact, that the specific heat of He-II varies as T^3 at low temperature and its excitation spectrum resembles with that of a well ordered crystalline solid indicate that He-II has an ordered arrangements of atoms. Over the last few years, Jain [4] has been working on this problem and developed successfully its microscopic theory consistent with microscopic as well as macroscopic uncertainty, volume exclusion and modified volume exclusion conditions. His theory also provides microscopic basis for the system to behave as a mixture of two fluid as envisaged by Landau [2]. It is this microscopic theory which forms the basis of our present investigation.

Chapter-I of the thesis reviews the important aspects of theoretical formulations and experimental studies on liquid ${}^4\text{He}$.

Chapter-II describes the salient aspects of the microscopic theory of a system of interacting bosons such as liquid ${}^4\text{He}$, as developed by Jain [4]. Jain's theory reveals that: (i) the system below certain temperature T_λ should behave as a homogeneous mixture of two fluid (ii) the superfluid transition is identified as an order-disorder transition of particles in their phase space followed by B.E. condensation of particles as $(q, -q)$ pairs in a state of their centre of mass momentum $K=0$; individual atom retains $\hbar k = h/2d$ momentum corresponding to zero-point energy. (iii) no state of the system corresponds to $k=0$ state of single particle hence the question of the existence of $k=0$ condensate in the system is far from reality. (iv) Particles in the phase below T_λ represent 3-d network of stationary matter wave (SMW) pairs $(q, -q)$ that modulate the probability of finding the particles in phase space. Below T_λ the SMW pair configuration is perturbed by the overlap of the wavepackets and the interatomic attraction and the particles develop a kind of collective binding energy identified as energy gap between normal and superfluid states and this gap is responsible for all the unique properties of superfluid (v) The relative positions of particles in phase space

is found to be $2n\pi$ ($n = 1, 2, 3, \dots$) and this fact is responsible for the phase coherence of particles and quantized vortices observed in He-II (vi) the system below T_λ defines a closed pack arrangement of the wavepackets of its particles that can be ascribed to have a symmetry such as hcp/fcc.

Chapter-III gives a detailed quantitative analysis of the thermal excitations of He-II. Using the microscopic theory as proposed by Jain [4,5], it was noted that the system is isotropic and is equivalent to a crystal with one particle per unit cell. It was further noted that the shear force among its particles is negligible and thus the transverse modes are absent. The phonon energy was concluded to follow a dispersion relation for a single atomic chain. Since the interatomic separation (d) is not rigidly fixed and the size of the wavepacket of a particle is momentum dependent, it has been argued that it should be a function of wavevector q and thus obviously the force constant (C) is also a function of q . Our study of the excitation spectrum based on these inferences is reported in this chapter. This includes the analysis of:

(i) the " q " dependence of (C) and (d) of the excited state configuration.

(ii) the anomalous nature of the thermal excitation spectrum

on a quantitative scale.

(iii) the inter-relationship between "C" and "d".

(iv) the pressure dependence of the roton energy and momentum.

(v) The interaction between the multimode and the single particle excitation, which leads to a hybridization.

(vi) The relationship between the Thermal Excitation spectrum and structure factor. Our theoretical results match with the experimental results to a very good approximation.

Chapter-IV gives the calculation of the first sound velocity as a function of temperature by assuming three possible structure of the system. The pressure dependence of the velocity of first sound at constant temperature has also been analysed. To understand the change in the strength of inter-particle interaction, we examined the variation of the force constant with pressure for wavevector $q = 0$. Calculation of the superfluid and normal density of He-II were done by using, what has been defined by Jain as the energy gap between the ground state of the system in superfluid and normal fluid configurations. These results have been used to obtain the velocity of II, III, IVth sound which have been found to agree with the experimental results to a good approximation.

Chapter-V present a critical analysis of the observed Raman spectrum of He-II. The origin of a number of unexplained peaks in the high resolution Raman spectrum of He-II are reported.

Chapter-VI gives some important concluding remarks pertaining to our investigation and provides a line of action that we plan to follow for further investigation of the system.

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CHAPTER: I

EXPERIMENTAL AND THEORETICAL STUDIES

OF LIQUID HELIUM-4

1.1 INTRODUCTION

Helium-4, known to exist in Sun's atmosphere since 1868, was discovered to exist on earth in 1895 by Ramsay [1]. It occurs in the atmosphere with a concentration of about 1 part in 200000 [1]. In 1908, Kamerlingh Onnes [2] obtained liquid ${}^4\text{He}$ having boiling point 4.2K at atmospheric pressure. It remains liquid even at 0K unless a pressure of about 25atm. is applied. However, it undergoes a liquid to liquid phase transition of second order at temperature $T=T_\lambda=2.17\text{K}$. At $T>T_\lambda$ the liquid behaves like a normal liquid and is referred as He-I. At $T<T_\lambda$ the liquid acquires the unique property of superfluidity which is characterised by zero viscosity [1,3,4] and is referred as He-II or superfluid ${}^4\text{He}$. Superfluidity has rightly been recognised as the manifestation of quantum nature at macroscopic level.

For about six decades, various properties of He-II have challenged and enlightened the scientific community. It has been playing a unsurpassable role of unravelling the intricacies of quantum principles. Liquid ${}^4\text{He}$ has, therefore, been extensively investigated. A large number of reseach papers, review articles and books have been written on this system. In the following we attempt to summarise its important properties and conclude on the present status of its understanding.

1.2 EXPERIMENTAL STUDIES OF HE-4

1.2.1 Density measurement: Measurement of the density of liquid helium as a function of temperature was done by Kamerlingh Onnes in 1911 [5]. The result exhibited a strange property of density maximum at 2.2K, which implies that the liquid exhibits negative expansion below 2.2K. More accurate measurements were performed confirming the existence of the density maximum in the neighbourhood of 2.2K. The density of liquid He as a function of pressure has been measured by Keesom and Keesom [6]. A well defined power law behaviour of superfluid density near the transition temperature was observed by Chan et. al. [7] by introducing disorder with the help of porous medium. Neutron scattering experiments were done by Herwig and Sokol [8] for normal fluid at 4.25K at 11 densities between 0.125 and 0.200gm/c.c and the variation of the kinetic energy per particle was studied. Niemela and Donnelly [9] calculated density from dielectric constant from the range 1.15K to 4.9K and also provided formula for absolute density measurement from the range 0K to 4.9K.

1.2.2 Dielectric constant measurement: In 1927 Keesom and Wolfke [10] observed that the dielectric constant shows a sudden jump in the vicinity of 2.3K, suggesting a liquid to liquid phase

transformation. Similar results were obtained by Grebenkemper and Hagen [11] at 9100 MHz by measuring the resonant frequency of helium filled microwave cavity. Chase et. al [12] measured the dielectric constant from the range 1.4K to 4.2K and showed that the polarizability is independent of temperature. The latest work on dielectric measurement was done by Niemela and Donnelly from the range 1.15K to 4.9K [9].

1.2.3 Measurement of surface tension: A jump in the surface tension was observed by Urk et. al. [13]. Atkins [14] showed that the surface tension is dominated by the surface modes called ripplons. The experimental verification of surface modes was done by Atkin and Narahara [15] by measuring the height of the liquid in a glass capillary tube. Edward et.al [16] verified Atkins theory by measuring surface tension below 0.3K. However the experimental results of Eckordt et.al [17] do not seem to agree with the theory proposed by Atkins. A lot of work on surface tension followed thereafter. The recent works are cited in the references [18-25]. Recent experiment [22] seem to show that below the λ -point the surface tension of liquid ^4He contains an additional contribution due to the distribution of the equilibrium superfluid order parameter. The low temperature surface tension of ^4He is calculated on the basis of microscopic

theory using excitation. The role of the excitations in surface tension calculation is clarified and it is found that only bulk excitation contribute to the surface tension and that the excitation can be ignored up to 2.2K [24]. Lu et.al [25] calculated the expression of surface tension by taking into consideration the finite size of the molecular superfluid helium.

1.2.4 *Measurement of specific heat:* A discontinuity in the specific heat (C_{svp}) of ^4He was noticed by Keesom and Wolfke in 1927 [10]. They measured the temperature dependence of the C_{svp} and observed a jump in the vicinity of 2.19K. The shape of the specific heat verses temperature curve resembles the shape of the letter λ and therefore the singular point observed in this curve is called the λ -point. At the λ -point no latent heat characteristic of a first-order phase transition was observed, indicating it to be a second - order phase transition. It is seen that the C_{svp} varies rapidly near the λ -point, as $\ln |T-T_\lambda|$. The possibility of such a logarithmic infinity appears to have been first suggested by Tisza [26]. The measurements approaching closest to the lambda line are those of sp.heat by Fairbank et. al. [27,28]. Empirically they showed that C_{svp} varies as

$$C_{\text{svp}} = -0.65 - 3.00 \log_{10} |T - T_\lambda|, \quad T > T_\lambda \quad \text{Joules. g}^{-1} \cdot \text{deg}^{-1}$$

$$C_{\text{svp}} = 4.55 - 3.00 \log_{10} |T - T_{\lambda}|, \quad T < T_{\lambda} \quad \text{Joules. g}^{-1} \cdot \text{deg}^{-1}$$

Several other determination of the specific heat under vapour pressure have since been made [29-32]. A recent work on C_{svp} of confined ${}^4\text{He}$ at T_{λ} was done by Nissen et.al [32].

1.2.5 Thermal Conductivity: Keesom and Keesom in 1936 discovered the unexpectedly high thermal conductivity of He-II. Its maximum attained at 1.9K has a value equal to $810 \text{ Cal cm}^{-1} \text{ sec}^{-1} (\text{K})^{-1}$ [33]. Other experiments studying the heat flow in He-II were performed by Allen and Jones in 1938 [34]. They discovered the so called Fountain effect (thermo - mechanical effect). In this experiment the increase of the temperature produces the pressure difference between bulb and reservoir. The fountain effect equation was derived first by London [35] and has been used to make accurate measurements of entropy of He-II and its variation with temperature and pressure [36]. Daunt and Mendelsohn [37] in 1939 discovered the mechanocaloric effect, - the inverse of the Fountain or the thermomechanical effect. This has been confirmed by Brewer and Edwards [38]. A lot of work on this interesting phenomenon has been carried out thereafter. Grant et.al [39] measured the transient heat transfer of He-II at a temperature of 2K under transverse magnetic field of 1.5T. The co-efficient of

thermal conductivity in thin and bulk ^4He , as function of temperature was measured by Um et.al [40]. Thermal conductivity of ^4He at SVP, confined in a glass capillary was measured by Kahn and Ahlers [41]. They showed that below T_λ the thermal conductivity becomes effectively infinite when the correlation length becomes small compared to the size of the confining holes.

1.2.6 Viscosity measurement: The measurement of the coefficiently viscosity (η) of He-II was done by Kapitza in 1938 by using a modified capillary flow method [42]. The upper limit estimated from these experiments shows that the η of He-II must be 10^4 times smaller than that of Hydrogen gas. η was also measured by Allen and Misener in 1938 by using an ordinary flow method [43]. They also found a vanishingly small value. Furthermore they observed that the velocity of flow is practically independent of the pressure difference at the ends of the capillary. However, the result obtained by using oscillating discs, vibrating wires and rotation viscometers [44] contradicts the result obtained by Kapitza [42] and Allen and Misener [43]. They found that below the λ - point the viscosity of He-II does not differ significantly from that of He-I showing that η does not vanish in He-II and this non-vanishing η value laid the foundation of the famous two-fluid theory. The recent works are as given in the references [45,40].

1.2.7 Propagation of sound : The velocity of first sound has been measured by determining the wavelength by Van Itterbeck et. al [46] and by a radar-pulse technique by Chase [47]. The phenomenon of second sound was first predicted by Tisza [48]. The present treatment was given subsequently but independently by Landau [49]. The second sound is essentially an entropy or temperature wave in which the entropy or temperature function plays an entirely analogous role to the density or pressure function in an ordinary sound wave. Different works of second sound are cited in the references [3] and very recently a work on second sound on superfluid filled porous media was done by Warner and Beamish [50] by using ultrasonic wave of frequency range 4 to 31 MHz. Third sound [51] is a surface wave on a He-II film, in which the superfluid oscillates parallel to the substrate, while the normal fluid is clamped because of its viscosity. The full theory of third sound is based on two-fluid hydrodynamics, augmented to include the interaction between liquid and vapour across the interface [52]. Measurement were also done by Rudwick [53] and the recent work on third sound was done by Sheldon and Hallock [54]. The fourth sound is a pressure wave in He-II inside a superleak, where the normal component is immobilised and only the superfluid is in motion. Different works on fourth sound are given in the reference [4].

1.2.8 *Experimental study of condensate:* The existence of Bose condensate has been believed to be the origin of superfluidity. It has been proposed by several workers that the neutron inelastic scattering measurement of $S(Q, \omega)$ at large Q should give a direct experimental evidence of the condensate [55]. Identically, measurement of surface tension and X-Ray diffraction are also considered for determining the existence of n_0 . An extensive review of these studies has been made recently by Glyde and Svensson [56] by covering several hundreds of research reports available in the literature. We will not go into the details of the experimental results available from this studies, however, it may be mentioned that these studies have been aimed at finding answers of the questions such as (1) does the dispersion of the excitations in the system at low q have anomalous nature (2) why do we not observe dramatic change in $S(Q, \omega)$ on passing through T_λ (3) why should the width and the central position of $S(Q, \omega)$ at large Q have periodic oscillations (4) why does $S(Q, \omega)$ at large Q show no evidence of sharp central component believed to be arising from scattering by zero momentum atoms. We find that the analysis of a wealth of experimental studies reported in this field provide answer to some of these questions, however, we also find that they leave with us many different set of puzzles to be addressed by future investigations. As such it is evident that the existence

of $p = 0$ condensate has not been proved beyond doubt. In fact it is not surprising because the result of the theoretical development (cf Chap. II of the thesis) conclude that $p = 0$ condensate is not expected to exist in the system at all. The particles gets condensed as pair in the state of their center of mass momenta $K = 0$. Individual particles retain $h/2d$ momentum that account for their zero point energy.

Thus many surprising and interesting properties discovered over the last several years awaits for a general theoretical explanation.

1.3 THEORETICAL STUDIES:

Frohlich in 1937 first suggested that the λ -transition is a special kind of order-disorder transition [57]. His model was however criticized by London [58], who proposed that the phenomenon is a manifestation of Bose-Einstein condensation - a consequence of Bose-Einstein statistics of non - interacting bosons [59,60]. London seems to have been guided by the fact that $T_{\lambda} = 2.17K$ and the temperature of Bose-Einstein condensation $T_{B.E} = 3.13K$ (calculated for liquid Helium density = 0.145gm/c.c) do not differ significantly and believed that a macroscopic fraction of ^4He atoms is locked into the state of zero momentum.

Using simple arguments related to the participation of particle in $p=0$ states in momentum dissipation and entropy contribution, it is revealed that the system should behave as if it contains two interpenetrating fluids (i) Superfluid (composed of condensed particles) which should have zero entropy as well as viscosity and (ii) normal fluid (composed of excited particles) which should have non zero values of entropy and viscosity.

The idea of the so called "Two fluid theory" of He-II was used by Tisza [61] to explain the properties of same. He considered the motion of He-II as some kind of turbulent motion because the velocity pressure dependence is more similar to turbulent than to laminar motion. The most important success of Tisza theory was the prediction of the existence of the temperature waves in He-II.

London's idea was next exploited effectively by Landau [62]. However, his theory, also called a two-fluid theory assumes the existence of two independent motions in He-II. These two motions occur without momentum transfer from one to another and treated the superfluid flow by expressing the macroscopic hydrodynamical variables like the density and velocity, as quantum mechanical operators. He further showed that the equations of motion for

these operators implied the continuity equation and Euler's equation for an ideal fluid. From the standard conservation laws, Landau showed that the motion of the gas of excitation (phonons and rotons) would be of the normal viscous type, governed by a Navier-Stokes equation. Landau's 1941 paper is undoubtedly the most influential single contribution to the development of the theory of He-II. In this paper, however, Landau rejected the view that the properties of an ideal Bose gas below its condensation temperature might have any thing to do with the behaviour of He-II. It is clear from the literature that this remained a matter of dispute for some time. Although Landau's model has recieved significant success in accounting for the peculiarities of He-II, however, it also has several shortcomings, inconsistencies and quantitative disagreements with certain experimental results. The model also encounters several paradoxial situation [59], viz., the rotational paradox: while the superfluid is not expected to participate into the rotation, the experiments reveal that it certainly does so, and the viscosity paradox: the η determined by using capillary flow, rotatory, and oscillatory viscometers is observed to have three different values.

Efforts have been made to reconcile with some of the weak points of Landau model. Putterman [59] remarked that the two

fluid model supplemented by Onsager [63] and Feynman [64] quantization (i.e circulation of the superfluid around the vortex line in term of integral multiple of h/m) has strong similarities with the Old Quantum theory in which Bohr-Sommerfield quantization was used to select the allowed states of an atom. As the old Quantum theory has shortcomings in that it did not take into account the wave particle duality, one naturally expects that Landau theory plus Quantization will have comparable shortcomings. In any case Landau Theory is a phenomenological model which cannot be an alternative for a unified microscopic theory. Making a speculative remark Putterman stated that the present Quantum mechanics lacks in necessary first principles for describing Superfluidity of He-II.

Bogoluibov [65] in 1947 demonstrated the connection between the microscopic theory of superfluidity and Bose-Einstein condensation. He considered a nearly perfect Bose-Einstein gas with degenerate condensation. On the assumption that the single-particle state of lowest energy is macroscopically occupied, this theory showed that the condensate would be depleted by the interactions and derived an excitation spectrum to that proposed by Landau [66].

Although the interaction between Helium molecules is comparatively weak, liquid ${}^4\text{He}$ cannot be considered as a "nearly perfect" Bose-Einstein gas. Thus the problem of the justification of the Landau spectrum on the basis of a microscopic theory remained open. This important problem was undertaken by Feynman [67,68]. He first used his path-integral formulation of quantum mechanics to confirm that a condensation would occur in a Bose system having strong inter-particle interaction. Secondly, arguing from the symmetry properties of the many boson wave function, he showed that (i) an excitation spectrum of the Landau type is a natural consequence. and (ii) there cannot be any low-energy excitation other than phonons in He-II.

In 1956, Feynman and Cohen [69] proposed a more flexible variational wave function that simulated the interaction between phonons. This yielded a low $E(q)$ in good agreement with experiments at SVP. They found the value of the roton energy as 11.5K.

Lee and Mohling [70] in 1959 examined the experimental data for the total cross-section for the inelastic scattering of cold neutrons in liquid He-II. They concluded that the projection of the angular momentum on the direction of the momentum p of the

roton is equal to zero. This means that the roton excitations have zero angular momentum and confirm that they do not have rotational characters.

Bogoliubov's theory emphasises the importance of a "degenerate condensate" for superfluidity. The idea was developed further by Onsager and Penrose [71] and by Bogoliubov [72,73]. Onsager and Penrose proved that Bose-Einstein condensation takes place in ^4He at absolute zero. They also proved that for a system with condensate $\langle \Psi(t,r) \rangle \neq 0$, where $\langle \Psi(t,r) \rangle$ is the mean value of the Bose operator $\Psi(t,r)$. This property of the system with condensate allowed Bogoliubov [73] and Hohenberg and Martin [74] to obtain independently the hydrodynamical equation from the microscopic theory. Such a derivation has helped to calculate from the microscopic theory the spectra of the elementary excitation at small momenta.

The hydrodynamic equation with viscous terms were derived in the Bogoliubov scheme by Galasiewicz [75,76] and Krasnikov [77]. Khalatnikov [78] assumed that the distribution function for elementary excitation in Helium satisfies a Boltzmann equation. Existence of the ODLRO (off-diagonal long range order), a criterion for the existence of long-range order [79] was not found

in one and two dimension [80].

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A number of many body methods varying widely in approach and underlying principle have been employed to develop the microscopic theory of He-II. The hard core repulsive part of the He-He interaction has been considered to pose serious difficulties in solving the Schrodinger equation of the system.

In a gas of non-interacting bosons, the ground state at absolute zero has all the particles in the same state with momentum zero. This macroscopic occupation of a particular state leads to difficulties in the application of many-body techniques to liquid Helium. Efforts to overcome these difficulties were initiated by Beliaev [81] and Hugenholtz and Pines [82]. However, exact results were obtained only for long wavelength region.

The classic work of Bogoliubov on the dilute weakly interacting gas is equivalent to the work of Beliaev [81] for small potential. The Bogoliubov approximation is therefore, a small V approximation. However, it is inconsistent with the known experimental results. Its great triumph is that it shows that if the potential is repulsive, the dispersion relation is linear with wave vector (q).

The Bogoliubov approximation [65] is applicable for sufficiently weak interaction for which first-order perturbation theory is adequate. Since it is impossible for two ^4He atoms to be at the same point at the same time the potential is certainly not weak at short distances. Brueckner and Sawada [83] developed a theory allowing for strong repulsive interactions by assuming that the liquid was dilute. Parry and Ter Haar [84] have estimated the error produced by this Bogoliubov approximation to be only about 3%. Calculations have been performed with this theory by Goble and Trainor [85] who used various hard-core radii and solved the equation.

Bycking [86] performed similar calculation, but allowing for all partial waves for Lennard-Jones potential with a hard-core radius of 2.6\AA . The calculated excitation curves were qualitatively similar to the experimental results.

Singh and Kumar [87,88] have extended the theory to include a weak attractive interaction in addition to the repulsive core. The attractive interaction is treated by first-order perturbation theory and the repulsive interaction by a T-matrix. All these theories give results which at low frequencies reduce to the Bogoliubov approximation with a modified form of potential.

Another approach to approximating the self-energy for liquid ${}^4\text{He}$ has been that of Tserkonikov [89,90], Pines [91,92], Etters [93] and of Cheung and Griffin [94,95] who have attempted to apply the same approximation as those inherent in the random phase approximation of an electron gas.

Several other theories of liquid ${}^4\text{He}$ have exploited the similarity between the λ -transition ${}^4\text{He}$ and Superconducting transition in metals by suggesting that there is a similar pairing in liquid ${}^4\text{He}$. In the original pairing theories of Valatin and Butler [96], Girardeau and Arnowitt [97], Luban [98], Kobe [99] and Brown and Coopersmith [100], a microscopic occupation of the zero momentum state was assumed and the Bogoliubov transformation was performed. The remainder of the Hamiltonian was, however, truncated so that it could be diagonalized in a similar manner to that used in the theory of superconductivity. However, this has not been justified. Recently pairing theories have been developed by Congilio et.al [101] and Evans and Imry [102], in which there is no macroscopic occupation of the zero momentum state, but an effective attractive interaction between the particles to produce a pair condensation. These theories are however, considered to be unrealistic.

A related but somewhat different formalism to that described above has been developed by Brandow [103,104]. He suggested that instead of using the many-body theory developed by Beliaev [81] and by Hugenholtz and Pines [82] it is preferable to treat Helium as a Fermi system with infinite spin degeneracy. The infinite spin degeneracy permits the condensation of all the particles into a single spatial state and has the advantage that the techniques developed by Goldstone [105] for Fermi system may be taken over directly to the ^4He .

A combination of the Transformation method (TM) [65,83] and the correlated basis-function approach (CBF) [105-110] which has been extensively used to study a strongly interacting N-body system, of interacting bosons has also been used to express the ground state [110-112]. The U-matrix theory [113] was used by Fung and Lam [114] to study several crucial features of liquid ^4He at 1.1 K, based on a model Hamiltonian which includes two particle interaction function.

Recently, however, Jain [115] discovered that one of the basic premises used (in one form or the other) in the theoretical formulations of different aspects of the system becomes inconsistent with the uncertainty principle particularly for

particles of momentum $p \leq h/2\lambda$. Jain, therefore, used a new approach to develop the long awaited microscopic theory which explains all peculiar properties of He-II. We sum up this theory in Chapter-II of this thesis.

1.4 SOME OF THE PECULIAR PROPERTIES OF HE-II

- (i) non-zero viscosity if measured through rotatory or oscillatory viscometers; mention may be made that even the results of these two measurements do not agree with each other.
- (ii) infinitely high thermal conductivity (about 10^3 times that of copper).
- (iii) singularities ($T = T_\lambda$) in the specific heat, volume expansion coefficient and dP/dT .
- (iv) thermomechanical and mechanocaloric effects.
- (v) negative volume expansion.
- (vi) unique property of flowing upward by itself along the walls of the container.
- (vii) quantized circulation having magnitude nh/m (where $n = 1, 2, 3, 4, \dots$).
- (viii) property to sustain the propagation of density oscillation (first sound), as well as the temperature oscillation (second sound).

- (ix) its calm and still nature in contrast with the nature of He-I which is greatly agitated by bubbles of vapours.
- (x) the anomalous nature of single quasi-particle excitations around the low values of wavevector q .

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CHAPTER: II

MICROSCOPIC THEORY OF SUPERFLUIDITY

OF HELIUM-II

2.1 INTRODUCTION

As a manybody system of interacting bosons, liquid ${}^4\text{He}$, which transforms from its normal state (He-I) to its superfluid state (He-II) on cooling through $T_\lambda = 2.17 \text{ K}$, has been a subject of exhaustive studies [1,2], particularly for its unique behaviour of He-II known as Superfluidity. This behaviour is believed to originate from the Bose-Einstein condensation (BEC) of ${}^4\text{He}$ atom to its ground state. Although numerous efforts have been made to develop the microscopic theory of the system by using various methods of treating strongly interacting particles [2], however, the desired theory could not emerge until recently when Jain used a new approach and successfully developed the long awaited theory [3]. Henceforth this theory would be referred to as the JAIN'S MODEL. The model provides microscopic basis for He-II to behave as a homogenous mixture of two fluids as envisaged by Landau [4]. In addition it also establishes some of the important ideas of London [1b], Putterman [1c] and the ψ - theory [1]. Pertaining to the failure of other theoretical formulations, Jain observes the following:

- (i) The assumption that the system possesses random distribution of its particle in phase space even in the low temperature phase is not justified.

(ii) As shown in this chapter, a single particle state does not exist even for a simple system of two particles. The existence of such a state is unjustified. Naturally one cannot believe in the existence of $p = 0$ condensate.

(iii) the definition of the hard core (diameter σ), as used in these formulations in constructing a pair wavefunction or in defining the scattering length etc, is a classical concept. It loses its utility particularly when the wave packet size, $\lambda/2$ (λ being the de Broglie wavelength of the particle) becomes larger than σ i.e when the quantum nature of the particles dominates over their classical character. Jain categorically concludes that the use of σ in defining the boundary condition on the pair waveform is not consistent with the basic principle of wave mechanical uncertainty, particularly for the states of low energy particles with $p < h/2\sigma$. Naturally, the theories based on such conditions cannot provide a right understanding of the ground state and hence the right physics of the system.

2.2 HAMILTONIAN AND BASIC ASPECTS OF THE SYSTEM

The Hamiltonian of a system of N interacting bosons such as ^4He atoms is written as

$$\mathcal{H} = - (\hbar^2/2m) \cdot \sum_i \nabla_i^2 + \sum_{i < j} V_{ij}(r_{ij}) \quad (1)$$

where $V_{ij}(r_{ij})$ represents the interaction between two bosons separated by distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. The interaction has two components: (i) short range repulsion which is identified as the hard core potential defined by $V_{ij} = \infty$ for $r_{ij} < \sigma$ (the hard core diameter of the atom) and zero for $r_{ij} \geq \sigma$, and (ii) a relatively long range (effectively not larger than few atomic separation) weak attraction. To proceed further Jain notes the following:

(1) Following the analysis of liquid ^4He by Huang et.al. [5], Woo [6] and Chester [7], the total attractive potential that an atom experiences from its neighbours is expected not to fluctuate much. It can be replaced by a constant negative external potential (that acts on individual particles). One is left with only the repulsive core to deal with. Evidently, within certain bounds (viz. the cavity formed by the neighbouring particles), an atom in liquid ^4He moves like a free particle. The course of the motion changes when it collides with the neighbouring atoms or the walls of the container. But after the collision, its free particle character is retained. This picture forms the starting point of Jain's model.

(2) Again, two particles in the system having any possible momenta k_1 and k_2 as observed in the laboratory frame see each

other as particles of equal and opposite momenta having magnitude of their relative momentum, $k=k_1-k_2$. In the frame attached to their centre of mass (CM), two particles are seen to form a pair of particles with momenta q and $-q$ ($q=k/2$). The wave mechanical study of a pair of such particles reveal that two particles always adopt the configuration $(q,-q)$ pair which moves with its CM momentum $K=k_1+k_2$ in the laboratory frame. Jain also concludes that the pair formation is an energetically favourable process. As such $(q,-q)$ pairs are of central importance to describe a system like ${}^4\text{He}$.

(3) A critical study of the wavemechanics of two hard core bosons reveals several important facts useful for better understanding of the N-particle system. The Schrodinger equation for a pair of hard core bosons can be written as

$$-\frac{\hbar^2}{2m} \left[\nabla_1^2 + \nabla_2^2 \right] \psi(r_1, r_2) + V(r) \cdot \psi(r_1, r_2) = E \cdot \psi(r_1, r_2) \quad (2)$$

The notation have their usual meaning; the interparticle interaction $V(r)$ is zero for $r=|r_1-r_2|>\sigma$ and infinity for $r\leq\sigma$. To deal with $V(r)$, other studies [8] use a boundary condition (BC), $\psi(r<\sigma) = 0$ and $\psi(r\geq\sigma) \neq 0$ or its equivalent (e.g. Jastraw type correlation function); the wavefunction $\psi(r)$ describes the relative motion of two particles. However, Jain [3] proposes to

use a different condition that the interparticle separation (d) satisfies $d \geq \lambda/2$ (λ = de Broglie wavelength of particles). He uses the fact that a particle in wave mechanics manifests itself as a wavepacket of size $\lambda/2$; as two hard core particles do not overlap, he assumes that their wavepackets should do likewise. If $\lambda/2 > d$, particles would experience mutual repulsion unless $d = \lambda/2$.

In a physically possible state, two particles always remain in the zone of $V(r) = 0$, the equation of motion of the pair (Eqn. 2) when transformed to the centre of mass coordinate system can be written as

$$-\left[\frac{\hbar^2}{4m} \nabla_R^2 + \frac{\hbar^2}{m} \nabla_r^2 \right] U^\pm(R,r) = E \cdot U^\pm(R,r) \quad (3)$$

with

$$U^+(R,r) = (\sqrt{2}/V) \cdot \cos(k \cdot r/2) \cdot \exp(iK \cdot R) \cdot \exp[-i(E)t/\hbar] \quad (4)$$

$$U^-(R,r) = (\sqrt{2}/V) \cdot \underline{\underline{\cos(k \cdot r/2)}} \cdot \exp(iK \cdot R) \cdot \exp[-i(E)t/\hbar] \quad (5)$$

where use is made of

$$U^\pm(R,r) = 1/(\sqrt{2}) \left[U_{\mathbf{k}_1}(\mathbf{r}_1) U_{\mathbf{k}_2}(\mathbf{r}_2) \pm U_{\mathbf{k}_2}(\mathbf{r}_1) U_{\mathbf{k}_1}(\mathbf{r}_2) \right] \quad (6)$$

and

$$U_{\mathbf{k}}(\mathbf{r}) = A \exp(i\mathbf{k} \cdot \mathbf{r}) \quad (7)$$

Where $R = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ represent, respectively, the

coordinates of the CM of the pair and the relative position of two particles. Similarly $K = k_1 + k_2$ and $k = k_1 - k_2$, represent, respectively, the momentum of CM and relative momentum of two particles. A critical analysis of $U^\pm(R,r)$ reveals the following:

(1) The probability amplitude for finding the two particles of relative momentum k to have a relative separation r is given by

$$|U^+(R,r)|^2 = 2.\cos^2(k.r/2) = 1 + \cos(k.r) \quad (8)$$

$$|U^-(R,r)|^2 = 2.\sin^2(k.r/2) = 1 - \cos(k.r) \quad (9)$$

which are independent of K . This shows that the probability depends only on k and r . Since $K = 0$ implies that $k_1 = -k_2 = q$ (say), the pair of particles in the frame attached to its center of mass adopt a $(q, -q)$ configuration with $q = k/2$. In the laboratory frame this pair is observed to move as a single entity having a plane wave motion of momentum K .

(2) Comparing the form of $U^\pm(R,r)$ with that of a well known stationary wave of sound or electromagnetic radiation, it was observed that $U^\pm(R,r)$ represents a kind of stationary matter wave (SMW) which modulates the probability of finding the particles in the phase space. The pair in the momentum configuration $(q, -q)$

is proposed to be known as SMW pair.

(3) It was suggested that a proper choice of $U^{\dagger}(R,r)$ that takes care of the hard core potential should correspond to a configuration in which two wave packets do not overlap. If the particles are considered to remain confined in two separate antinodal regions, then the condition of no overlap of wavepackets is satisfied.

(4) Neither of $U^{\dagger}(R,r)$ is a eigenvector of momentum and energy operators of a single particle thus revealing that a single particle state does not exist~~s~~ even for a simple two free particle falling in the quantum regime. Obviously the presumption of the existence of a state ($p = 0$) which at $T \leq T_{\lambda}$ is occupied by many particle is far ^{from} reality.

2.3 STATE WAVEFUNCTIONS OF THE SYSTEM.

A state wavefunction $\Phi(1,2,..N)$ of a system of N-particles is written as the product of N wavefunctions, treating the particles as separate entities. It is stated that, although, two particles in their quantum regime lose their identity as independent particles and form $(q, -q)$ pairs, nevertheless one can use this methodology to write $\Phi(1,2,3,..N)$ for a state of the system as it

offers a simple method of addressing a particle in $(q, -q)$ configuration as a separate entity. Since each particle in the $(q, -q)$ pair is a representative of the pair it is expressed as $U(R, r)$. In addition for a free particle enclosed in an enclosure, there exist two fields: one expressed by $[A \exp(ik' \cdot r')]$ and the other by $[A \exp(ik'' \cdot r'')]$ representing the reflection of the former from the walls of the container. The superposition of these two fields results in a kind of SMWs that represent the eigenstates of a particle in a box. In view of these observations, he first analysed a system of two particles for developing a better understanding of large system of N particles.

To account for the additional reflected plane wave fields, the Hamiltonian of the pair is expressed by

$$\mathcal{H}(1,2) = -\frac{\hbar^2}{2m} \cdot \sum_{j=1}^2 \nabla_{r_j}^2 = -\frac{1}{2} \cdot \sum_{j=1}^2 \left[\frac{\hbar^2}{2m} \nabla_{r'_j}^2 + \frac{\hbar^2}{2m} \nabla_{r''_j}^2 \right] \quad (10)$$

Where prime (') and double prime (") indices refer, respectively, to the actual and reflected fields. Using the CM coordinate system, one has

$$\mathcal{H}(1,2) = -\frac{1}{2} \cdot \sum_{j=1}^2 \left[\frac{\hbar^2}{4m} \nabla_{R_j}^2 + \frac{\hbar^2}{m} \nabla_{r_j}^2 \right] \quad (11)$$

Here the notations have their usual meaning. The terms in the square bracket of Eqns. (10), and (11) refer to a j -th particle (as independent entity) expressed obviously, by $U(R,r)$ type pair waveform that can be obtained by using the superposition of $u_{\mathbf{k}_j}(\mathbf{r})$ and its reflection $u_{\mathbf{k}'_j}(\mathbf{r})$. This gives

$$U_{\mathbf{K}_j, \mathbf{k}_j}(R, r) = \frac{\sqrt{2}}{V} \cdot \cos(\mathbf{k}_j \cdot \mathbf{r}_j / 2) \cdot \exp[i(\mathbf{K}_j \cdot \mathbf{R}_j)] \cdot \exp[-i(E_j + e_j)t / 2\hbar]. \quad (12)$$

having energy eigenvalue

$$\varepsilon_j = E_j + e_j = \frac{\hbar^2}{8m_j} K_j^2 + \frac{\hbar^2}{8m_j} k_j^2 = \frac{\hbar^2}{4m_j} [k_j'^2 + k_j''^2] = \frac{\hbar^2}{2m_j} k_j^2 \quad (13)$$

where $\mathbf{K}_j = \mathbf{k}'_j + \mathbf{k}''_j$, $\mathbf{k}_j = \mathbf{k}'_j - \mathbf{k}''_j$ and $k'_j = k''_j = k_j$. As revealed by Eqn.(13), the representation of a particle by pair waveform does not change its energy. Here is noted that $U(R,r)$, representing a particle of the pair can, in principle, be obtained by using the superposition of any two of the four plane waves. The number of possible ways in which four plane waves can be used to construct a pair waveform are: (1'1''), (1'2''), (1'2'), (2'1''), (2'2'') and (1''2''); in these abbreviated notations for the pairs, the integer numbers refer to particles involved in the construction of a $U(R,r)$. The possible ways in which these $U(R,r)$ defines different statefunctions (with same energy eigenvalue) of two particles are:

$\psi_1 = (1', 1'')(2', 2'')$, $\psi_2 = (1', 2'')(2', 1'')$, and $\psi_3 = (1', 2')(1'', 2'')$ and that all the four plane waves are included in each of the three possible eigenfunctions as they should. Each of these ψ functions has a form such as

$$\psi_1 = \left[\frac{2}{V} \cdot \prod_{j=1}^2 \cos(k_j \cdot r_j / 2) \right] \cdot \frac{1}{\sqrt{2}} \left[\sum_{\mathcal{PK}} \left\{ \frac{1}{V} \cdot \prod_{j=1}^2 \exp[i(K_j \cdot R_j)] \right\} \right] \cdot \exp \left[\sum_j -i(E_j + e_j)t / 2\hbar \right] \quad (14)$$

Here $\sum_{\mathcal{PK}}$ refers to the sum of permutations of K values over all particles and the three different ψ enumerated above take care of the permutation of k values. The energy eigenvalue for each ψ is found to be

$$E = \varepsilon_1 + \varepsilon_2 = \frac{\hbar^2}{2m} (k_1^2 + k_2^2) \quad (15)$$

A general function that represent a state of the pair is given as

$$\phi(1,2) = \frac{1}{\sqrt{3}} [\psi_1 + \psi_2 + \psi_3] \quad (16)$$

Again it is mentioned that a pair waveform such as $(1', 1'')$ generated from the superposition of the plane wave of particle 1

and its own reflection represents a case of self interference (SI), and $U^+(R,r)$ appears to be the correct waveform to represent such situation because the hard core potential does not operate in this situation and the waveform need not vanish at $r = 0$, while the other cases such as $(1',2')$, $(1',2'')$, etc. represent the states of two particle interference (TPI), and one may prefer to use $U^-(R,r)$ to represent the situation because the waveform is expected to vanish at $r = 0$ as two particles can not sit over each other. But as the particles are identical, one finds no way to distinguish between a SI and a TPI situation. This again envisages the equivalence of $U^+(R,r)$ and $U^-(R,r)$ and one may use either $U^+(R,r)$ or $U^-(R,r)$ to keep a single frame of observation for all particles.

For a system of N particles in a container there are $2N$ plane waves. The number of ways in which these plane waves can be used to construct $U(R,r)$ representing N independent particles of the system are $N(2N-1)$. Using these $U(R,r)$ one can construct $\mathcal{N} = 1.3.5.7\dots(2N-1) = 2N!/2^N \cdot N!$ different statefunctions having same energy eigenvalue. Each one of these \mathcal{N} statefunctions has the form

$$\Psi(1,2,3,\dots,N) = \left[\left(\frac{2}{V} \right)^{N/2} \cdot \prod_{i=1}^N \text{Cos}(k_i \cdot r_i / 2) \right].$$

$$\left[\left(\frac{1}{N!} \right)^{1/2} \sum_{\mathcal{F}_K} \left\{ \left(\frac{1}{V} \right)^{N/2} \prod_{i=1}^N \exp[i(\mathbf{K}_i \cdot \mathbf{R}_i)] \right\} \right] \cdot \exp[-i \sum_{i=1}^N (E_i + e) t / 2\hbar] \quad (17)$$

The corresponding energy eigenvalue is

$$E = \sum_{i=1}^N \varepsilon_i = \sum_{i=1}^N \frac{\hbar^2}{8m} [K_i^2 + k_i^2] = \sum_{i=1}^N \frac{\hbar^2}{2m} k_i^2 \quad (18)$$

Obviously, the complete wavefunction representing a state of the system should be expressed by

$$\Phi(1, 2, 3, \dots, N) = (1/\sqrt{\mathcal{N}}) \cdot \sum_{i=1}^{\mathcal{N}} \Psi_i(1, 2, 3, \dots, N) \quad (19)$$

2.4 ORDER-DISORDER IN PHASE SPACE

To understand the role of the wave nature of particles in the evolution of the system with decreasing T it is noted that: (i) the particles in the system can have $\lambda/2 \leq d$ (where d = the nearest neighbour distance and $\lambda = 4\pi/k = 2\pi/q$), and (ii) in a system of constant particle density (i.e. constant d) the value of $(d - \lambda/2)$ decreases with decreasing T (i.e. increasing thermal de Broglie wavelength, λ_T). At certain temperature T_c (expression to be derived at a later stage), when $d - \lambda/2$ vanishes at large, k motions of all particles get freezed into zero point motions with $q = q_0 = \pi/d$ and energy $\varepsilon_0 = \hbar^2/8md^2$. Evidently, the system moves from a state of $\lambda/2 \leq d$ to that of $\lambda/2 = d$. While the former state corresponds to the relative phase positions of particles ϕ

$(=kd) \geq 2\pi$ which defines a random distribution of particles in the phase space, the latter state corresponds to $d = 2\pi$ defining an ordered state of particles in phase space. This implies a kind of transformation at $T = T_c$. With all k_j being equal to $2q_c = 2\pi/d$, this transformation makes all Ψ_j appearing in Eqn. (19) identical and $\Phi(1,2,3,\dots,N)$ attains the simple form of Ψ (cf Eqn. 17) which is a product of two functions dealing with k and K motions of particles separately. It is interesting that all the N (macroscopically large number) microstates of the system with decreasing T slowly merge into one state at $T = T_c$. This reveals a way to identify oneness of the system. Replacing all k_j in Eqn. (17) by $2q_c$, one have

$$\Phi(1,2,3,\dots,N) = \Phi_o(q_o; r_o, r_1, r_2, \dots, r_N) \cdot \Phi_e(K_1, K_2, \dots, K_N; R_1, R_2, \dots, R_N) \quad (20)$$

$$\text{with } \Phi_o(q_o; r_o, r_1, r_2, \dots, r_N) = \left(\frac{2}{V}\right)^{N/2} \left[\prod_{j=1}^N \text{Cos}(q_o r_j) \right] \cdot \exp[-i.N\varepsilon_o t/h] \quad (21)$$

$$\text{and } \Phi_e(K_1, K_2, \dots, K_N; R_1, R_2, \dots, R_N) = \frac{1}{\sqrt{N!}} \sum_{\mathcal{PK}} \left\{ \left(\frac{1}{V}\right)^{N/2} \prod_{j=1}^N \exp[i(K_j \cdot R_j)] \right\} \cdot \exp[-i.(\sum_j E_j) t/h] \quad (22)$$

and since the two functions Φ_o and Φ_e of the product defining $\Phi(1,2,3,\dots,N)$ Eqn. (20) deal with k and K motions of particles separately they can be considered to describe two separate

components of the system and the system can be regarded as their homogeneous mixture. The component described by $\Psi_0(q; r_1, r_2, \dots, r_N)$ would have zero entropy because it represents the ground state of the system where all particles are in the single state of $q = q_0$ and $\varepsilon = \varepsilon_0$. Further, since the particles in this state are trapped in the antinodal regions of stationary matter waves, they do not cross each other. They can move in the order of their locations and implies that the relative motions of particles cease to exist. Evidently, the fluid described by $\Psi_0(q; r_1, r_2, \dots, r_N)$ is not expected to possess any viscosity for its capillary flow. This fluid can, therefore, be identified as superfluid.

As one of the two possibilities, the process of excitation can take a particle to its higher energy states identified as the states of particle trapped in the cavity formed by neighbouring particles. These are the states of k motions and their energy is estimated to be $(nhq_0)^2/2m$ by assuming that the allowed values of q to a good approximation are nq_0 (with $n = 2, 3, \dots$). However, these are a kind of localised single particle excitations of energies $\approx (n^2 - 1)\varepsilon_0$ much higher than $k_B T$ for all $T \leq T_c$. Consequently, they do not contribute significantly to the thermodynamic properties of the system below T_c .

As another possibility a particle may be excited from its ground state configuration $(q_0, -q_0)$ expressed by $U_0(r) = A \cdot \cos(q_0 r)$ to $(q_0 + \Delta q, -q_0 + \Delta q)$ configuration described by

$$U_0(R, r) = A \cdot \cos(q_0 r) \cdot \exp(iKR) \quad (23)$$

where $K = 2\Delta q$, and $\Delta q = n\pi/L$ ($n=0,1,2,\dots$, and $L =$ size of the container). Since Δq can be infinitely small, corresponding motions would also have very low energy and a kind of correlation among such motions lead to collective motions such as phonons. This follows from the fact that particles in the system complying with $\lambda = 2d$ define a closed pack arrangement of their wavepackets, and the system is seen to have a kind of symmetry (not a rigid structure). This agrees with Landau's view [4] that He-II is more like a solid than a liquid. Using this aspect of atomic arrangement with inter-particle forces, we not only find that the qualitative nature of the excitation spectrum resembles with that envisaged by Landau but also conclude that it matches quantitatively with the experimentally observed spectrum in case of He-II [9]. As such, the excitation spectrum basically originates from K motions and $\Psi_e(K_1, K_2, \dots, K_N; R_1, R_2, \dots, R_N)$ represents a kind of gas of excitations such as phonons, rotons, etc. which account for the total entropy and other thermal properties of the

system. This may, obviously, be identified as the normal fluid. Further, since these quasi-particles move randomly they can produce nonzero viscosity.

2.5 IMPORTANT INFERENCES OF THE THEORY

Some of the important inferences of the theory are given below:

i). As the reference of each particle appears in both $\Phi_o(q_o; r_1, r_2, \dots, r_N)$ and $\Phi_e(K_1, K_2, \dots, K_N; R_1, R_2, \dots, R_N)$, all particles participate in both superfluid and normal fluid components at every stage.

ii). Since $\Psi(1, 2, 3, \dots, N)$ (Eqn. 19) describing a state of the system the at $T > T_c$ cannot be expressed as a product of two independent functions the behaviour of the system should be like a single component fluid as observed for liquid ^4He .

iii). Using the basis of Eqn. (23), $\Phi_o(q_o; r_1, r_2, \dots, r_N)$ for the flowing superfluid can be shown to transform as Φ_f given by

$$\Phi_f = \Phi_o(q_o; r_1, r_2, \dots, r_N) \cdot \text{Exp} [iK_f \cdot \sum_1^N R] \quad (24)$$

which not only resembles with the postulated waveform, $\psi(R) = \phi_0 \cdot \text{Exp}[iS(R)]$ [1e, 10], but also testifies that superfluid velocity v_s can be obtained from, $v_s = (\hbar/2m) \cdot \nabla S(R)$ with $S(R) = K_i \cdot \sum_i R_i$; note that $2m$ appears for m because K_i defines the CM momentum of a pair. This aspect may also provide a basis for the validity of ψ theory [10] for accounting the properties of He-II.

iv). Since the ground state of the system is characterised by all $k_j = 2q_0 = 2\pi/d$ and all $K_j = 0$, and the freezing of all k_j at $2\pi/d$ occurs at $T = T_c$, it is evident that the onset of particles (as SMW pairs) falling into their $K = 0$ state should start immediately as T falls below T_c . As such the transformation can also be identified as a BEC of particles as SMW pairs in the state of their $K = 0$.

v). To a good approximation T_c can be equated to the temperature equivalent (T_0) of the ε_0 characterised by $\lambda/2 = d$. Therefore, using $\lambda_T = h/\sqrt{(2\pi m k_B T)} = 2d$, we have

$$T_c \approx T_0 = h^2/8\pi m k_B d^2 \quad (25)$$

For liquid ^4He , this gives $T_c \approx 1.3 \text{ K}$ [3,11] which agrees closely with experimentally observed $T_\lambda = 2.17\text{K}$. In fact when necessary

correction is made for the thermal energy present in the K motions of the particles, T_c is found to fall very close to 2.17K [3,11].

vi). Since the system below T_c is a closed pack arrangement of the wavepackets of its particles, one finds that $\Phi_0(q; r_1, r_2, \dots, r_N)$ defines a kind of 3-D network of macroscopic SMW extending from one end of the system to the other without any discontinuity. This vindicates London's view that superfluid state of liquid ^4He , should be represented by a macroscopic wavefunction [1b] and this reveals in one way a kind of oneness of all the particles as envisaged in BEC state of the system [12].

vii). As $\Phi_0(q; r_1, r_2, \dots, r_N)$ vanishes at the boundaries of the system, ρ_s should vanish identically. This agrees with the experimental results pertaining to the velocity of third sound in the thin films of He-II [1e].

viii). Particles below T_λ have quantum correlations described by a potential [3],

$$U_{ij}^s = -k_B \frac{U_0}{\sigma} \ln[2\cos^2\{(\alpha + \phi)/2\}] \quad (\text{with } \phi = 2qr) \quad (26)$$

(where $\alpha = 0$ for U^+ and $\alpha = \pi$ for U^-)

which, has its minimum ($-k_B T_c \ln 2$) and maximum ($= \infty$) values at periodic phase positions, differing by $\Delta\phi = 2n\pi$ (with $n = 1, 2, 3$, etc.). Since U_{ij}^s increases as $C\omega^2$ ($C = \text{constant}$) for small change in ϕ around a point of its minimum, it generates a force $-2C\delta\phi$, which triggers order-disorder of particles in phase space at T_λ , and restores particles at $\Delta\phi = 2n\pi$ (with $n = 1, 2, 3$, etc.). The latter aspect reveals the origin of phase coherence of particles and quantized vortices of observed in He-II which have so far been understood in terms of a phenomenological argument by Feynman [13].

ix). The fact U_{ij}^s restores particles at $\alpha + 2qr = 2n\pi$ ($n=1, 2, 3, \dots$), not only reveals the interdependence of q and r but also concludes that the particles below T_λ should exhibit oscillations of their phase positions which can be expressed in terms of the oscillations of their q and r coordinates. This implies the existence of phonons as well as a new kind of quantum quasiparticle representing a phononlike wave of the *Oscillations of Momentum* (proposed to be known as OMON). The omon is an anti-phonon quasi-particle. The phase and group velocities of low q excitations are found to be $V_p = V_g = \sqrt{\pi} \cdot h/2md$ which gives ≈ 227 m/sec which compares very well with experimental value ranging between 220 - 237m/sec [1a].

x). When $\lambda/2$ tends to cross d with T moving below T_c , the wavepackets of neighbouring particles have an overlap because increase in d is constrained by interparticle attraction. This perturbs the U^+ waveform of each particle around its nodal points and hence its energy, ε_0 . Considering a pair of particles and following the standard method dealing with similar situation, he also finds that the energy of perturbed states become $\varepsilon_0 \pm |v|$; where $|v|$ is the magnitude of expectation value of interatomic potential due to overlap of wavepackets. $|v|$ could better be replaced by $|v(T)|$ as the overlap may depend on T . The state of lower energy ($\varepsilon_0 - |v(T)|$) represents a kind of bonding (bound pair) state while that of ($\varepsilon_0 + |v(T)|$) an anti-bonding (unbound pair) state. Thus the overlap and interatomic attraction lead to an additional binding between two particles. Since this happens to all particles, the ground state energy falls from $N\varepsilon_0$ (at $T = T_c$) to its new value $N\varepsilon_0 - N|v_N(T)| = N\varepsilon_0 - E_g(T)$; note that $|v_N(T)|$ may differ from $|v(T)|$ obtained for an isolated pair. When the system moves to this state, the wavepackets have increased size depending on $|v_N(T)|$. This forces the system to expand with decreasing T , as exhibited really by liquid ^4He [1a]. The expansion, however, needs energy to work against inter-particle attraction. Incidentally, the system at $T \leq T_c$ has small number, $N_e(T)$, of particles in the states of higher energy such that the

excitation wavelength $\lambda_e < \sigma$. Such particles behave as classical entities devoid of quantum correlations with other particles. When these particles with decreasing T fall to the ground state they release an additional energy, $\Delta\epsilon(T)$, ($k_B T \cdot \ln 2$ per particle) for their quantum correlations and have

$$\Delta\epsilon(T) = [N_{\uparrow}(T) - N_{\downarrow}(T)] \cdot k_B T \cdot \ln 2 \quad (27)$$

This energy available for expansion decides the extent of overlap and hence the $E_g(T)$. This gives $E_g(T) = \Delta\epsilon(T)$ and also have

$$E_g(T) = \frac{Nh^2}{4m} \cdot (d_I - d_{\uparrow}) / d_{\uparrow}^3 \quad (28)$$

Calculation for liquid ^4He , to a good approximation [3], gives $E_g(T) = \Delta\epsilon(T)$. The net loss of energy is $\Delta\epsilon(T) + E_g(T) = 2E_g(T)$ of which $\Delta V_g(T) = |E_g(T)|$ is restored back as an increased potential energy (= work done against the interatomic attraction) of particles forced to move away from each other by expanding wavepackets). $\Delta V_g(T)$ is a kind of self energy of particles which depends on their $\lambda/2$ or q values; it makes phonon propagation possible. $\Delta V_g(T)$ increases from $\Delta V_g(T) = 0$ to its maximum value at $T = 0$ and serves as a source of necessary energy for collective motions that could, therefore, be observed even at $T = 0$. He also

notes that the system is in a peculiar state of equilibrium in which particles are held at higher potential than that in N-state but the net energy, $N\varepsilon_0 - 2E_g(T) + \Delta V_s(T) = N\varepsilon_c - E_u(T)$, is lower than $N\varepsilon_0$. $E_g(T)$ identified as an energy gap between normal and superfluid states implies that particles in the superfluid phase have a kind of collective binding and the entire system behaves like a single molecule. However, this binding does not change the fluid like behaviour of the system since $E_u(T) \ll N\varepsilon_c$. The fact that $\varepsilon_0 \approx 4\text{K}$ obtained for liquid ${}^4\text{He}$ from this theory is lower than its 14K [6] value of conventional theories presuming $p=0$ condensate, revealing that the ground state configuration obtained is more favourable.

The stability of superfluid state is broken only when $E_g(T)$ energy is supplied from outside. Thus equating the flow energy and $E_g(T)$, the upperbound of critical flow velocity (v_c) was obtained to be equal to $\sqrt{[(2E_g(T)/Nm)]}$; using Eqn.(14) he got $v_c(T_\lambda) = 0$ to $v_c(T=0) \approx 9 \text{ m/sec}$ for liquid ${}^4\text{He}$. These results agree excellently with experimental results for He-II, e.g. $v_c = 2\text{m/sec}$. for a film of $\approx 25 \text{ \AA}$ thick and about $\sim 13\text{m/sec}$. for a orifice of $\approx 1\mu\text{m}$ diameter [14]. It was further noted that the appearance of quantized vortices can make the flow viscous even for lower v .

xi). The creation of temperature difference $\Delta T = T_x - T_y$ (with $T_x > T_y$) and/or pressure difference $\Delta P = P_x - P_y$ (with $P_x > P_y$) between two points X and Y in the system produces difference in $E_g(X)$ and $E_g(Y)$ and a state of inequilibrium. Consequently, phonons from X and omoms from Y flow, respectively towards Y and X to achieve equilibrium. For small ΔT and ΔP , the equation of state is

$$E_g(X) = E_g(Y) + S\Delta T - V\Delta P \quad (29)$$

Where S is the entropy and V is the volume of unit mass of the system. Using $E_g(X) = E_g(Y)$ for equilibrium, we have $S\Delta T = V\Delta P$. When this condition is used for capillary flow method of measuring viscosity (performed at $\Delta T = 0$) it gives $\Delta P = 0$ implying that the system behaves like superfluid of zero viscosity. Similarly in the experiments for measuring thermal conductivity \mathcal{K} (performed at $\Delta P = 0$) we have $\Delta T = 0$ which means that the system should have $\mathcal{K} = \infty$. In other experiments where non-zero ΔT (or ΔP) is maintained, we should observe $\Delta P = S\Delta T/V$ (or $\Delta T = V\Delta P/S$) in equilibrium. As such these experiments reveal that the system is a superfluid of high thermal conductivity that exhibit thermomechanical and mechanocaloric effects.

xii). For the first time, the theory finds that the specific heat

(C in J/Mole.K) of the system should exhibit logarithmic singularity as observed in case of liquid ${}^4\text{He}$ and have [3],

$$C = -A \ln(|T - T_\lambda|/T_\lambda) + B \quad (A = 5.28 \text{ and } B = -12.9) \quad (30)$$

The experimental results for liquid ${}^4\text{He}$ reveal $A \approx 5.355$ and $B \approx -7.77$ for $T > T_\lambda$ and $A \approx 5.100$ and $B \approx 15.52$ for $T \leq T_\lambda$ [1a]. The agreement of his result with these A values speaks of the accuracy of Eqn. (30). The theory do not expect an agreement with the values of B as Eqn.(30) is not the total C of the system.

xiii). Using the statefunction Eqn.(20), the single particle density matrix, $\rho(R-R')$ was obtained as,

$$\rho(R-R') = \left[\frac{N_0}{V} + \frac{1}{(2\pi)^3} \int N_K \text{Exp}[iK \cdot (R-R')] \cdot dK \right] \cdot \frac{2}{V} \cos^2 [q \cdot (r-r')/d] \quad (31)$$

Here $q \cdot (r_i - r'_i) = 2n\pi + q \cdot (r_i - r'_i)$ with $q = q_0 = \pi/d$. While the first term in square bracket is the number density of particles in the condensate characterised by $K = 0$ and the second term represents the correlation of two particles with CM at R and R', the remaining term represents the microscopic variation of density in closed pack of wavepackets. Using the fact the K motion energy of a single particle is $\hbar^2 K^2 / 8m$, the second term was shown to be

equal to $\text{Exp}(-2\pi|R-R'|^2/\lambda_T^{*2})$ with $\lambda_T^* = h/\sqrt{[2\pi(4m)k_B T]}$. It was noted that $\rho(R-R')$ does not vanish as $R-R' \rightarrow \infty$ particularly for low T phase where the number of particles (N_0) condensed into the state of $K=0$ as SMW pairs is non-zero. Naturally, there exists a non-zero value of off diagonal long range order among the particles in the system below T_λ .

2.6 CONCLUDING REMARKS.

The microscopic theory of liquid ^4He (a typical example of interacting bosons) as developed by Jain uses a new school of thought for the first time. The conventional thought uses certain premises shown to be inconsistent with the wave mechanical uncertainty; it also presumes the existence of $p = 0$ condensate which, however, violates the excluded volume condition as shown by Kleban [15]. The conventional thought, naturally, fails to reveal correct information about the ground state and other low energy states and hence the right understanding of the behaviour of the system. Since the conventional thought has been used to develop the understanding of the system over the last sixty years, the new school of thought developed by Jain naturally face resistance in reaching a stage of its acceptability. However, we decided to use Jain's model because it explains almost all properties of He-II. We are happy to note that Jain's model has now made a break

through. The important aspect of the Jain's theory is that the formation of $(q, -q)$ pairs of particles is an energetical favourable process. It originates from quantum correlation which under the influence of inter - particle interactions bind the two particles below T_λ . This binding differs from the binding of two electrons in a Cooper pair in the sense that the attraction of ${}^4\text{He}$ atoms is their natural property and it turns to be the collective attraction of all particles in the system. The theory concludes phase coherence and non - zero off diagonal long range order (ODLRO) below T_λ . This theory not only vindicates the elegant phenomenology developed by Landau [4] but also provides microscopic basis for certain aspects such as the vanishing of ρ_s at the boundaries of the system and existence of quantized vortices necessary to supplement the model for complete and correct description of the system. This also vindicates the important ideas of London [1b] on a superfluid state, and answers several intriguing questions raised by Putterman [1(c)]. It may be concluded, that, the model provides a sound footing for explaining many properties of ${}^4\text{He}$ in the microscopic scale and Jain's model provides for the first time a unified basis for understanding the system in 3-, 2- and 1-D. The theory also provides a right direction to understand the physics of the systems of hard core identical particles including liquid ${}^3\text{He}$,

neutron stars, atomic nuclei, superconductors, etc. It is going to make a revolutionary change in our understanding of the physics of even two particles in a box.

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CHAPTER: III

A STUDY OF THE THERMAL EXCITATION SPECTRUM

OF HELIUM-II

ABSTRACT

The excitation spectrum of liquid ${}^4\text{He}$ has been obtained theoretically by using structural configuration revealed from the microscopic theory developed by Jain. The anomalous nature of the phase and group velocities at low q has been analysed quantitatively by considering the variation of force constant (C) and the interatomic separation (d) with q . The behaviour of the Thermal Excitation Spectrum at $q > q_0$ has been investigated to explain the origin of plateau modes in terms of a kind of Fermi Resonance of interaction energy 4.5K . The pressure dependence of roton energy and position is also analysed by considering the roton as a coupled mode of two phonons. We find that the Feynman's relation between excitation energy and structure factor in its modified form obtained by Jain also explains the observed spectrum of He-II.

3.1 INTRODUCTION

The study of the thermal excitation spectrum of He-II started way back in 1941 when Landau [1] described the properties of He-II in terms of quasiparticle elementary excitations. An approximate form of the dispersion law of these excitations was established in 1947 by Bogolubov [2] in the theory of weakly interacting Bose gas and by Landau [3] on the basis of the analysis of experimental data on thermodynamics of liquid ^4He . Connection of the structure factor of ^4He with the spectrum of elementary excitation was determined by Feynman [4] and the same result was obtained by Pitaevskii [5] on the basis of quantum liquid hydrodynamics.

In 1961, Henshaw and Woods [6] measured the dispersion curve for the excitations in He-II by using neutron inelastic scattering and found that its nature agress with Landau's predictions. Despite this similarity, however, the agreement of the observed dispersion curve with the theoretical spectrum of quasiparticles in liquid helium has been a complicated problem.

A large number of research reports on the NIS spectra of He-II under different experimental conditions have been published [7-11]. The wealth of experimental results and related information thus collected has been recently reviewed by Glyde and

Svensson [12]. The typical nature of the experimentally observed spectrum is shown in Fig. 3.1 where names of different modes as used in the literature have been indicated in the caption to facilitate the discussion. The spectrum (cf curve A) is found to have qualitative agreement with the spectrum predicted by Landau.

In 1968, Cowley and Woods [13] also discovered a higher energy branch of the elementary excitations of He-II by using NIS technique. The new branch, also depicted in Fig.3.1 by curve-B, is almost flat with energy ≈ 22 K upto $q \approx 2.3 \text{ \AA}^{-1}$; it more or less follows the free particle energy dispersion, i.e. $E(q) = \hbar^2 q^2 / 2m$, beyond this point [12].

The three points of specific importance are identified by their energy ($E(q)$) and wavevector (q) coordinates as (Δ_0, q_0) , (Δ_1, q_1) , and (Δ_2, q_2) , on the low energy branch of the elementary excitations (Curve-A, Fig.3.1). They are respectively known as roton, maxon, and plateau modes. They play an important role in deciding various properties of He-II.

However it may be mentioned that the real description of the dynamics representing a roton/maxon/plateau mode in terms of the motions of the ${}^4\text{He}$ atoms was not understood until recently when a

report by Jain [14] has concluded the basic nature of the atomic dynamics representing not only the regions of these specific modes but the entire dispersion curve of He-II. Accordingly, the dispersion curve can be divided into five segments as done in Fig.3.1. While the segment-1 arises due to collective motions greatly resembling with the phonons in the crystalline system, segment-2 representing the region of the so called rotons arises due to motions that could be described by waveform resulting from the superposition of two phonon waves of equal and opposite group velocities. The segment-3 and segment-5 represent, respectively, the free particle motion with $E(q) \approx \hbar^2 q^2 / 2m$, and the multiphonon modes with $E(q)$ remaining almost constant at $\approx 22K$. Segment-4 is a consequence of an interaction between free particle motion and the multiphonon modes leading to considerable mixing of these modes when the dispersion curves representing these motions tend to cross around $q = 2.5 \text{ \AA}^{-1}$.

One of the interesting aspects of this spectrum is that its phononlike dispersion exhibits anomalous behaviour (in the range $q=0$ to $q \approx 0.6 \text{ \AA}^{-1}$) in the sense that group velocity (V_g) and phase velocity (V_p) of the phonons have positive gradient with q [12,15,16].

Several efforts have been made to derive the observed spectrum using microscopic formulations [1,17-23]. However, we note that : (i) the basic nature of the different excitations in terms of atomic motions and (ii) the anomalous nature of the phonon spectrum are yet to be understood. The basic difficulty originated from the fact that the arrangement of the atoms in the ground state of He-II has not been known. Like He-I (the normal phase of ^4He), He-II being also a liquid phase has always been considered to have random distribution of atoms in configuration space as well as phase space. However, certain experimental facts do not agree with this picture. In this context we note that the excitation spectrum of He-I differs significantly from that of He-II though the interatomic separation and the interatomic interactions in the two phases do not differ significantly. In view of this, it is obvious to think that the atomic arrangements of the two phases should differ in symmetry and structure and this difference should be responsible for the significant difference of their excitation spectrum. Here we may mention that : (i) Landau [1] also believed that He-II is more like a solid rather than like a normal liquid, (ii) Specific heat of He-II at low temperature varies as T^3 and (iii) the nature of the experimentally observed first order spectrum of He-II ranging from $q=0$ to $q \approx 2\pi/d$ (at this limiting value of q the excitation size becomes as small as

the size d of the interparticle separation of He atoms) matches closely with the nature of the phonon dispersion of a crystalline solid. These points not only corroborate that He-II should be a solid like system but also reveal that it should have an orderly arrangement of atoms. This is also revealed by the fact that hard core ^4He atoms in He-II experience a kind of additional repulsion originating from the zero point energy, a consequence of the wave nature of particles [24,25]; it is a well known fact that particles with repulsive interaction always arrange themselves at equal interparticle separation defining an orderly arrangement of a close packed system of hcp/fcc symmetry.

Jain [25] used these aspects of He-II to understand its observed excitation spectrum at a qualitative scale, and argued that the major parts of the spectrum could be understood in terms of: (i) phonons in a mono-atomic chains of ^4He where interatomic separation d and hence the interatomic interaction constant (C) are considered to change smoothly with phonon wavevector q and (ii) nearly free motion of single particle. The q point where the nature of the excitation has a transition from the former to that of the latter, corresponds to the q of what are popularly known as rotons. Mixing of nearly free motions of single particle and the multiphonon modes of excitation in the q ranging from ≈ 2.1 to

2.5\AA^{-1} and energy $E(q) \approx 22K$ also modifies the dispersion. In this chapter we first examine the variation of force constant (C) and the interatomic separation d with q that explains the phonon spectrum of He-II and its anomalous nature at a quantitative scale. In the following analysis we also examine the strength of mixing between multiphonon excitation and free motions of single particle, to account for the observed spectra for q ranging from 2.1 to 2.5\AA^{-1} .

3.2 EXCITATIONS IN HE-II AND THEIR ANALYSIS

3.2.1 Phonon like Excitation.

Excitations with $q < q_r$ (segment 1 of the dispersion curve, Fig 3.1) are rightly identified to be phononlike. This follows from the fact that the He-II is a close-packed system of the wavepackets representing the ${}^4\text{He}$ atoms [cf. Chapter II]. The wavepackets obviously have spherical shape of diameter $\lambda/2$ (where λ is the de Broglie wavelength of the particle). These wavepackets have equal diameter $\lambda/2 = d$ in the ground state of the system.

Now we note that the shear force among the atoms in He-II is negligibly small, the transverse modes are not expected. Further since He-II is an isotropic system, the three branches of the

longitudinal modes must also be identical. To a good approximation, therefore, the phonon dispersion $E_{\text{ph}}(q)$ is expected to resemble with dispersion of a monoatomic linear chain of atoms with equal separation, and we have

$$E_{\text{ph}}(q) = \hbar/k_B \sqrt{4C/m} \sin|(qd)/2| \quad (1)$$

Here $E_{\text{ph}}(q)$ is expressed in Kelvin, While d represents the lattice constant of the chain, C is a constant of potential representing the interaction between the two nearest ^4He atoms; other notations have their usual meaning. We note that d in He-II, being a close packed system of wavepackets, cannot be as rigidly fixed as in crystalline solids because an increase in energy/momentum of the particles leads to a decrease in the wavepacket size and vice-versa. Eqn. (1) would, therefore, be valid to a lower order of approximation. It is natural to think that with the amount of additional energy/momentum shared by the particles from the energy/momentum of the excitation the wave packet size of each particle would decrease and the particles in the excited state would come nearer to each other. Consequently, we have smaller d and higher C as q of the excitation increases. This implies that the parameters d and C of the chain of atoms used to define the state of excitation of a phonon are, respectively descending and

ascending functions of q . Thus to a better approximation, we have

$$E_{\text{ph}}(q) = \hbar/k_B \sqrt{4C(q)/m} \sin|qd(q)/2| \quad (2)$$

Jain [25] used this relation to qualitatively explain the anomalous nature of $E_{\text{ph}}(q)$.

In order to examine the validity of this explanation at quantitative scale, we followed the following steps :

(1) The values of V_p , V_g and $E_{\text{ph}}(q)$ for certain values of q were measured from the experimental curve reported in ref. [12,16,8]. These values are tabulated in Table 3.1 (columns 1,3 and 5).

(2) Using equation 2, the best possible values of $E_{\text{ph}}(q)$, $V_p = E_{\text{ph}}(q)/q$ and $V_g = \partial E_{\text{ph}}(q)/\partial q$ which are consistent with the experimental values were obtained theoretically for different q values by using proper values of $d(q)$ and $C(q)$ with the help of the Lotus Package for computer analysis. To calculate the values of $d(q)$ and $C(q)$, we have used the relations as given below for lower values of q

$$C(q) = \frac{\hbar^2 \pi}{4md(q)} \quad (3)$$

$$d(q) = \frac{2\pi}{(2\pi/3.709 + q/2)} \quad (4)$$

While Eqn. (3) is a result of Jain's theory, Eqn. (4) is obtained from $q = 2\Delta q = 2 [(2\pi/d(q) - (2\pi/d(0))]$ and $d(0)$ for He-II is 3.709.

The values of $C(q)$ and $d(q)$ for higher values of q were obtained through the method of iteration that gives $E_{ph}(q)$, $V_p(q)$ and $V_g(q)$ values agreeing closely with experimental results.

The theoretical values obtained are tabulated in Table 3.1 (columns 2,4, and 6).

(3) The variation of $C(q)$ and $d(q)$ as a function of q are tabulated in Table 3.2 and depicted in Figs. 3.2 and 3.3.

The variation of C and d with q was found to be more or less linear in nature as depicted in the figures; having $C = 2.74$ for $d = 3.709$ for $q = 0$ and $C = 5.46$ for $d = 2.85$ for $q = 1.1$. The accuracy of this analysis is evident from the facts that: (i) the theoretical values of $E_{ph}(q)$, V_p and V_g calculated through Eqn. 2 match very well with the experimental values as shown in Figs. 3.4 - 3.6. (Table 3.1) and (ii) the model also accounts for the

anomalous nature of the phonon dispersion at quantitative scale. It is further corroborated by the fact that the variation of $C(q)$ with the change in $d(q)$ as shown in Fig.3.7 is found to be nearly linear (a reasonable and acceptable nature) except in the small range of $d(q)$. It is observed that $C(q)$ at smaller values of $d(q)$ is nearly constant. This indicates that the interaction potential is nearly parabolic in nature. However, for $d(q)$ increasing beyond this small range, $C(q)$ decreases linearly indicating that the ${}^4\text{He}-{}^4\text{He}$ potential flattens in agreement with a nature normally expected.

The expression for the excitation energy given by Eqn. 2 agrees very well up to the region marked as segment 1 in the dispersion curve shown in Fig. 3.1, proving the q dependence of d and C .

3.3 MIXED MODES OF EXCITATIONS

For $q > q_0$, where the excitation wavelength λ_{ex} becomes shorter than the interatomic separation, the total energy and momentum is possessed by the lone particle. Naturally the mode of excitation in this region would resemble to a good approximation with free particle motion having energy dispersion $E(q) = \hbar^2 q^2 / 2m^*$ where m^* is the effective mass of the ${}^4\text{He}$ atom. However the parabolic dispersion so expected can be modified by mixing of this

mode of motion with other modes of motion, such as multiphonon modes. We therefore believe that the excitations of He-II in the range of $q = 2.1$ to 2.5 \AA^{-1} are the mixed modes of multiphonons of energy $\approx 22 \text{ K}$ (nearly independent of q) and the free particle motions.

Ruvalds and Zawadowski [26]. explained the observed dispersion in this range as a resonance of two rotons with single particle spectrum. Using Green function technique they showed that an interaction between these two motions can produce hybridization and splitting of one particle spectrum into two distinct branches. We agree with this account to a certain extent. However, since the energy of two rotons ($\approx 17.2\text{K}$) remains below the energy of the multiphonon - mode branch (19K to 24K) it is more appropriate to identify the multi-mode branch as a combination mode of a maxon and a roton, which is expected to have $\approx 22\text{K}$ energy. We notice that the multi-mode branch (segments 5 and 5') having energy $\approx 22\text{K}$ and single particle dispersion $E = \hbar^2 q^2 / 2m^*$ (segments 3 and 3') as shown in Fig.1 would cross at $q \approx 2.5 \text{ \AA}^{-1}$ if no mixing is present between them. Using the kind of Fermi resonance interaction of energy = 4.5K , we find a very good agreement between our results and experimentally observed dispersion [19,26,27] revealing that the multiphonon-mode

branch deviates from its characteristic curve (segment 5) to follow the (segment 3'), while the single particle dispersion (segment 3) deviates to go along the multi-mode branch (segment 5'). High degree of mixing of two modes leading to what has been described as their hybridization by Ruvalds and Zawadowski [26] is noted in the region enclosed by a rectangle (see Fig. 3.1).

Our calculation follow the standard theory of accidental degeneracy of two modes. If Ψ_1 and Ψ_2 are the eigenfunctons of the (i) multiphonon mode having energy independent of q and (ii) the single particle motion having energy $= \hbar^2 q^2 / 2m^*$.

$$\text{we have } H_0 \Psi_1 = E_1 \Psi_1 \quad (5)$$

$$\text{and } H_0 \Psi_2 = E_2 \Psi_2 \quad (6)$$

where H_0 is the Hamiltonian.

Considering the mixing of these modes due to the accidental degeneracy, the Hamiltonian gets modified because of a perturbation term. The new Hamiltonian can be written as $H = H_0 + H'$. The term H' represents the perturbation.

The wavefunction of the mixed state can be represented by $\psi = a\psi_1 + b\psi_2$ where a and b are the constants. Using ψ and H and also the orthonormality of ψ_1 and ψ_2 , we obtain

$$a(E_1 - E) + b\varepsilon = 0 \quad (7)$$

$$a\varepsilon + b(E_2 - E) = 0 \quad (8)$$

where $\varepsilon = \langle i|H|j\rangle$

From equation (7) and (8) we can find the value of E^+ and E^- given by

$$E^+ = \frac{1}{2} \left[E_1 + E_2 \right] + \frac{1}{2} \left\{ \left[E_1 - E_2 \right]^2 + 4 \left[\varepsilon \right]^2 \right\}^{\frac{1}{2}} \quad (9)$$

$$E^- = \frac{1}{2} \left[E_1 + E_2 \right] - \frac{1}{2} \left\{ \left[E_1 - E_2 \right]^2 + 4 \left[\varepsilon \right]^2 \right\}^{\frac{1}{2}} \quad (10)$$

In Table 3.3, q is the wave vector, E_1 stands for the multiphonon-mode branch of He-II, and E_2 gives the energy of the single particle branch at different values of q ; ε stands for the interaction energy. E^+ and E^- are energies of the resulting dispersion in the range of q under discussion. We notice that our calculated results of E^+ and E^- are in good agreement with experimental value of E^+ and E^- [19,26,27] depicted in Fig. 3.8.

3.4 PRESSURE DEPENDENCE OF ROTON POSITION AND ENERGY

The roton has been interpreted by Feynman [28] as a vortex ring of the smallest possible size. This view has been further developed by Williams [29] recently. On the other hand Chester [30] interpreted the roton as being an atom moving fast through the sea of other atoms. This latter view is in line with the interpretation of Glyde and Griffin [31], who viewed the roton as being a dressed single particle excitation. However our analysis does not agree with these interpretation and it follows from section 3.2.1 that the dispersion of the excitation in the system follows Eqn. (2) where the force constant and the interparticle separation depends upon q and also has a mirror symmetry (as shown in Fig. 3.9) at $q = \pi/d$. However as q crosses $2\pi/d$ the system offers another configuration of the chain whose collective motion could equally well be excited and as such excitation follows curve B of the Fig. 3.9. But, as shown in the figure we then have two different configuration of the chain that may participate in the collective modes of motion in the system. We note that the excitation of one of the chain possesses positive group velocity (cf Fig. 3.9) while the other has negative group velocity (cf Fig. 3.9). As such it appears that the excitations for $q > 2\pi/d$ must be the coupled modes of excitation in both the chains and the energy should be the sum of two excitations.

Following this we find that the roton minimum should have a q value given by

$$q=q_0 = \frac{1}{2} \left[\frac{2\pi}{d} + \frac{2\pi}{c} \right] \quad (11)$$

The energy should be twice the energy of the cross over point (C) of the two dispersion curves (cf Fig.3.9)

$$\text{i.e } \Delta_0 = 2 E_{\text{ph}}(q) \text{ at } q = q_0 \quad (12)$$

We use this relation to find the pressure dependence of q_0 and Δ_0 and it is interesting that our result agree very well with experimental results [32,33]. Table 3.4 shows the values of q_0 calculated and Table 3.5 and Table 3.6 shows the value q_0 and Δ_0 calculated us and by others by using different techniques (cf Figs 3.10 and 3.11). This gives the basic character of the motion responsible for roton minimum.

3.5 EXCITATION SPECTRUM AND STRUCTURE FACTOR

The connection between the structure factor and the spectrum of elementary excitation of liquid ^4He was determined by Feynman [4] by using a microscopic formulation.

Feynman's relation relates the energy of excitation $E(q)$ with

that of free particle motion $\varepsilon(q)$ and the structure factor $S(q)$ by

$$E(q) = \varepsilon(q)/S(q) = \hbar^2 q^2 / 2mS(q) \quad (13)$$

The value of $E(q)$ so obtained showed a qualitative agreement with the observed experimental spectrum of He-II but its magnitude was found to be higher by a factor of two. To achieve a quantitative agreement, Feynman and Cohen [15] considered a kind of back flow but however a good agreement could not be obtained at high q .

Using a SMW pair as the basic unit of the system as proposed by Jain [cf. chapter II], the free particle motion is modified by changing m by $2m$ and the new relation for the free motion is thus $\hbar^2 q^2 / 4m$, the excitation energy is now rewritten as,

$$E(q) = \varepsilon(q)/S(q) = \hbar^2 q^2 / 4mS(q) \quad (14)$$

The variation of $E(q)$ as a function of q is studied in this section by putting the corresponding value of $S(q)$, the results obtained are shown in Table 3.7 and is found to agree very well with the experimental values obtained by neutron scattering (Fig 3.12) and thus proves the pair formation as proposed by Jain.

Table 3.1: Experimental and theoretical values of V_p , V_g and E_{ph} for different values of q

q	expt.	theor.	expt.	theor.	expt.	theor.
\AA^{-1}	V_p^*	V_p	V_g^{**}	V_g	E_{ph}^{***}	E_{ph}
	m/sec	m/sec	m/sec	m/sec	K	K
	1	2	3	4	5	6
0.0	237.7	238.0	237.7	238.3	00.00	00.00
0.1	241.3	243.7	238.5	248.4	01.69	01.86
0.2	245.3	246.9	240.5	251.4	03.48	03.78
0.3	248.7	247.9	242.5	248.2	05.54	05.69
0.4	247.3	247.0	240.5	239.9	07.27	07.55
0.5	242.6	244.9		189.4	09.54	10.15
0.6	233.9	236.7		161.0	10.60	10.86
0.7	221.3	224.4		128.8	12.31	12.01
0.8	206.6	209.4		095.7	12.87	12.81
0.9		193.8		063.9	13.69	13.34
1.0		179.1		031.5	13.79	13.69
1.1		164.6		000.8	14.46	13.84

* see Ref. 12

** see Ref. 16

*** see Ref. 8

Table 3.2: Values of Force Constant C and Interatomic Separation d as a function of wave vector q

q \AA^{-1}	$C(q)$ dyne/cm	$d(q)$ \AA
0.0	2.74	3.709
0.1	3.08	3.602
0.2	3.45	3.502
0.3	3.85	3.407
0.4	4.29	3.317
0.5	4.78	3.232
0.6	5.08	3.166
0.7	5.26	3.098
0.8	5.34	3.025
0.9	5.38	2.95
1.0	5.42	2.9
1.1	5.46	2.85

Table 3.3: Accidental degeneracy of the single particle excitation and the multiphonon mode at about $q = 2.5 \text{ \AA}^{-1}$.

q \AA^{-1}				theor.		expt.	
	E_1 K	E_2 K	ε K	E^+ K	E^- K	E^{+*} K	E^{-*} K
2	22	09.34	4.5	23.43	7.90	23.7	9.3
2.1	22	09.88	4.5	23.49	8.40	22.8	10.3
2.2	22	11.56	4.5	23.67	9.89	23.7	11.7
2.3	22	14.34	4.5	24.07	12.26	24.7	13.4
2.4	22	18.22	4.5	24.99	15.23	26.6	16.1
2.5	22	23.23	4.5	27.15	18.07	29.9	19.0
2.6	22	29.34	4.5	31.48	19.86	35.1	19.9
2.7	22	36.56	4.5	37.84	20.72	41.8	20.5

* see Ref. 19

Table 3.4: Values of roton position (q_0) as a function of density.

Press. atm.	Density gm/cc	d Å	$2\pi/d$ Å ⁻¹	$2\pi/\sigma$ Å ⁻¹	q_0 Å ⁻¹
01	0.1462	3.568926	1.760753	2.220494	1.990624
05	0.1522	3.521398	1.784518	2.220494	2.002506
10	0.1584	3.474841	1.808427	2.220494	2.014461
15	0.1636	3.437629	1.828004	2.220494	2.024249
20	0.1681	3.406676	1.844613	2.220494	2.032553
25	0.1722	3.379421	1.859489	2.220494	2.039992

Table 3.5: Theoretical and experimental values of roton position.

Density gm/cc	wavevector(q_0) \AA^{-1} theor.	wavevector(q_0) [*] \AA^{-1} expt.
0.1462	1.990624	1.9316
0.1522	2.002506	1.9526
0.1584	2.014461	2.0053
0.1636	2.024249	2.0474
0.1681	2.032553	2.0684
0.1722	2.039992	2.0947

* see Ref. 32

Table 3.6: Theoretical and experimental values of roton Energy.

Density gm/cc	Δ_o (roton energy) K theor.	Δ_o^* (roton energy) K expt.
0.1484	8.3058	8.6842
0.1521	8.0000	8.4737
0.1579	7.5520	8.1052
0.1637	6.9882	7.6842
0.1679	6.8000	7.3158
0.1721	6.6116	7.0000

* see Ref. 33

Table 3.7: Calculation of $E(q)$ through structure factor $S(q)$

q	$S(q)^*$	$E(q)$	$E(q)^{**}$
\AA^{-1}		theor.	expt.
		K	K
0.0	0.001	0.00	0.00
0.2	0.032	3.96	3.48
0.4	0.070	7.20	7.27
0.6	0.113	10.02	10.6
0.8	0.165	12.19	12.87
1.0	0.228	13.78	13.79
1.2	0.325	13.91	14.15
1.4	0.470	13.09	13.38
1.6	0.680	11.82	12.00
1.8	1.02	09.97	9.49
2.0	1.23	10.20	9.34
2.2	1.20	12.65	11.77
2.4	1.08	16.73	16.07
2.6	1.03	20.59	17.57
2.8	1.00	24.59	18.31
3.0	0.97	29.11	18.41
3.2	0.94	34.17	19.34
3.4	0.94	38.58	19.72
3.6	0.94	43.25	20.08

* see D. G. Henshaw, Phys. Rev. 119, 14(1960)

** see Ref. 8

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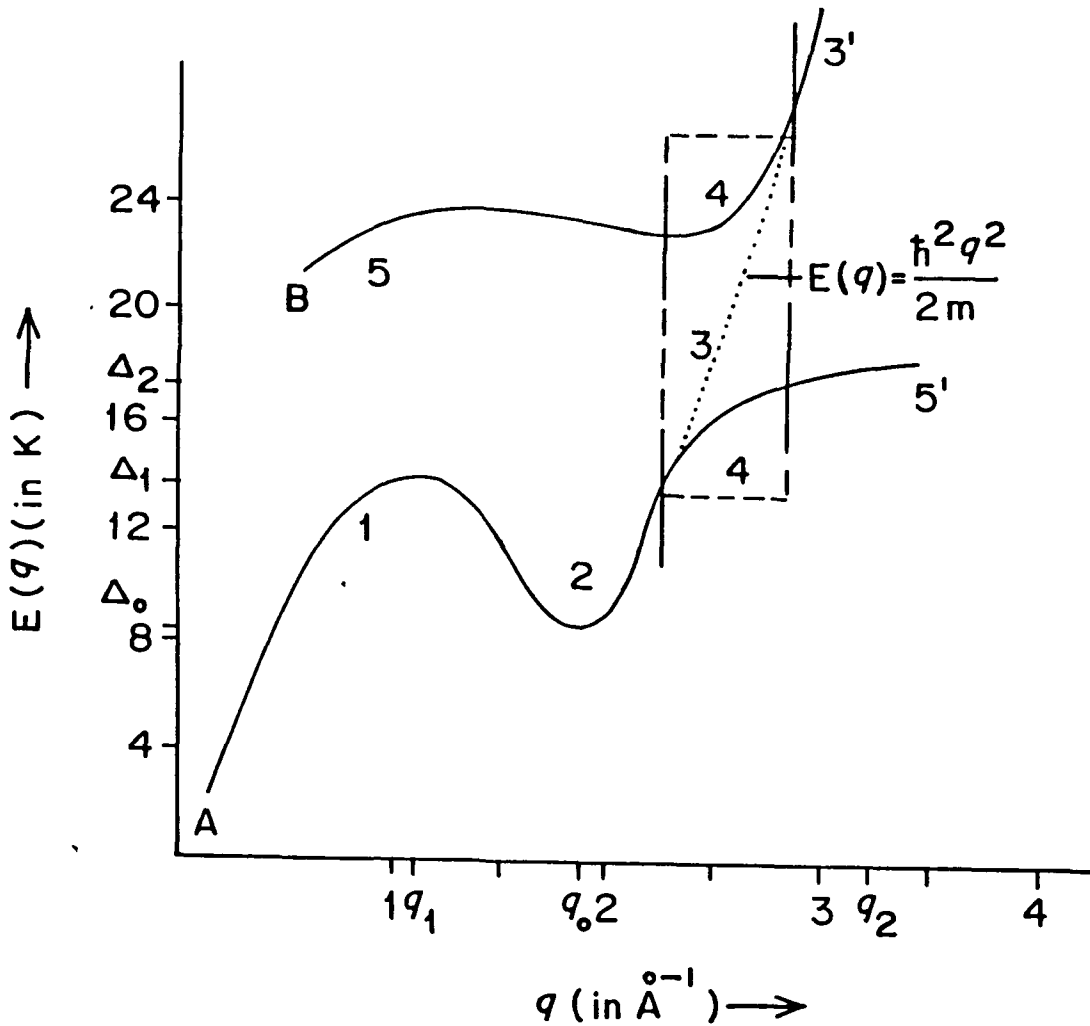


Fig.3.1: The Typical nature of the Thermal Excitation Spectrum as observed experimentally by the neutron inelastic scattering. The different modes as used in the literature are as given in the segments - (1) phonons, (2) roton minimum, (3 and 3') free particle motion (4) as a consequence of an interaction between the free particle motion with the multiphonon mode and (5 and 5') multiphonon mode. (Δ_0, q_0) , (Δ_1, q_1) and (Δ_2, q_2) stands respectively for roton, maxon and plateau mode.

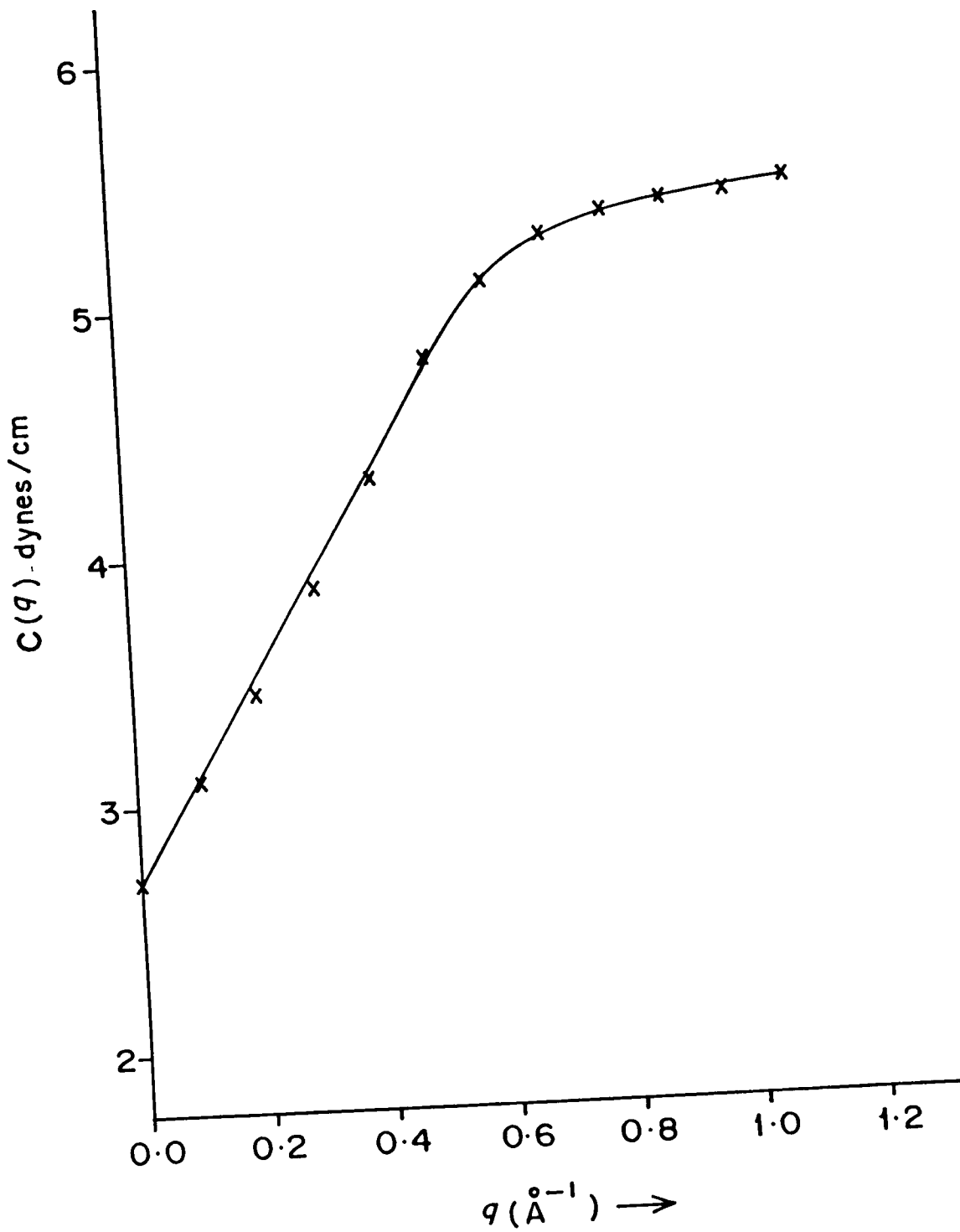


Fig.3.2: Variation of $C(q)$ (force constant) as a function of q (wave vector).

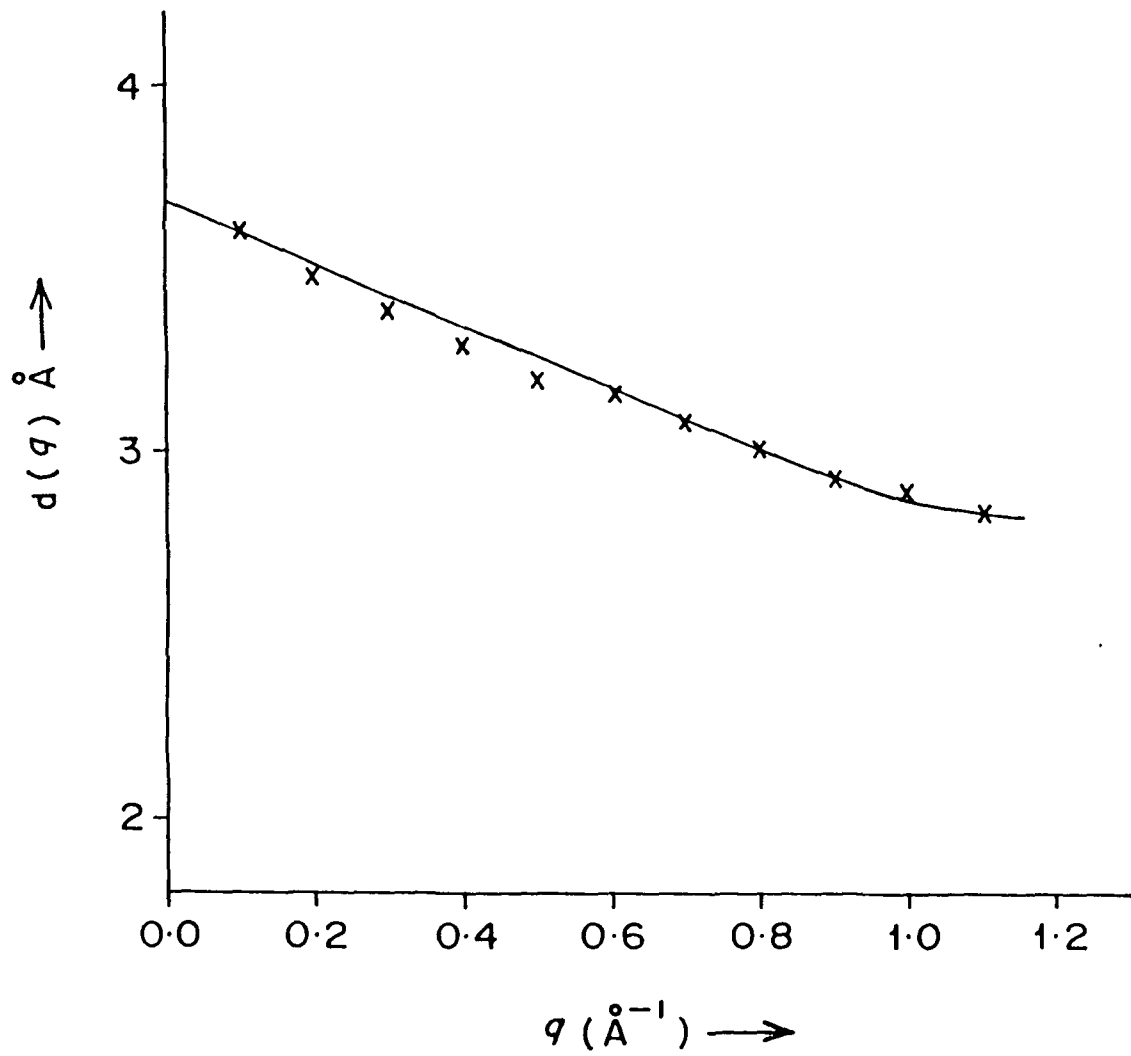


Fig.3.3: Variation of $d(q)$ (interatomic separation) as a function of q (wave vector).

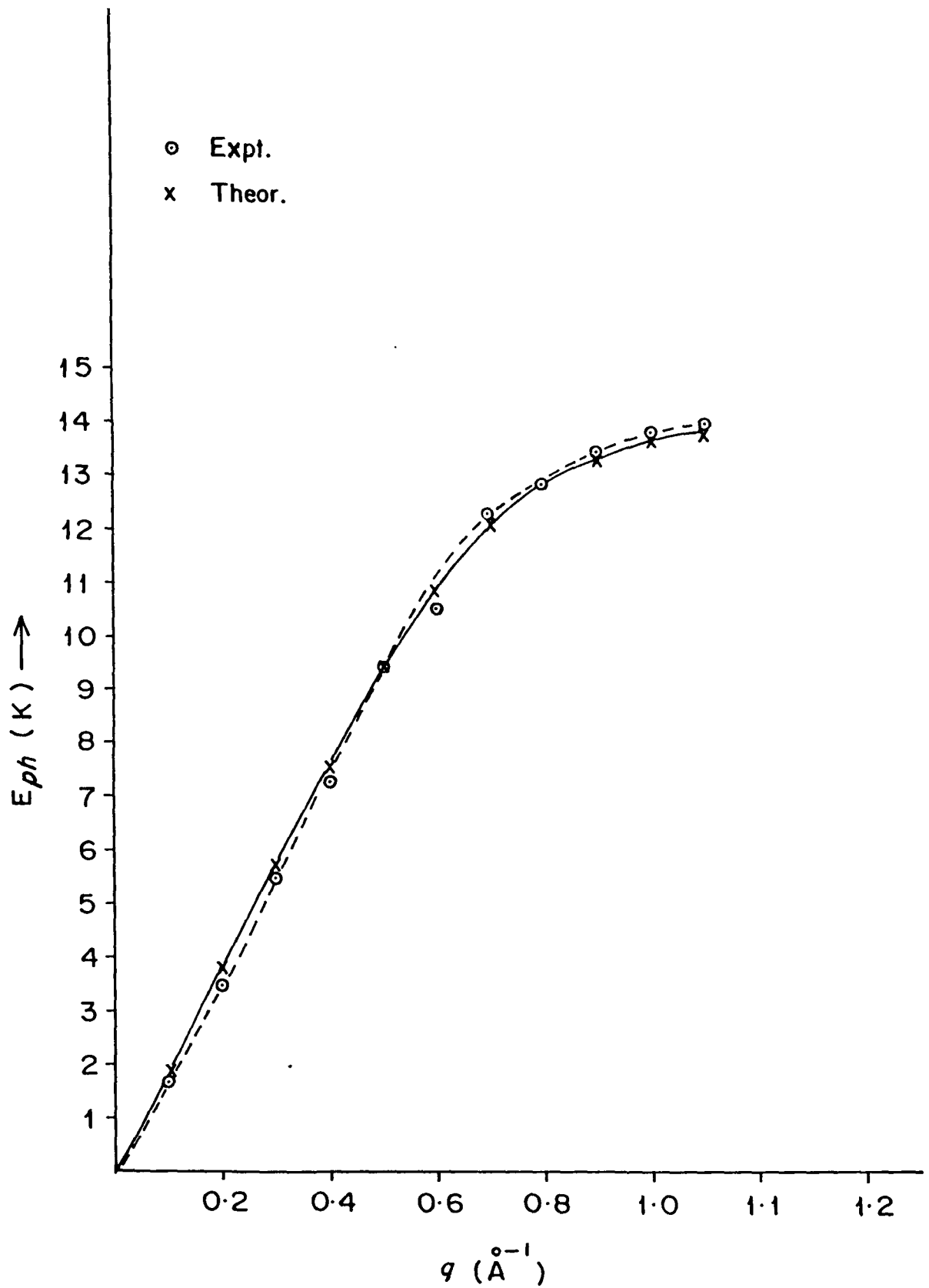


Fig.3.4: Comparison of Energy E_{ph} obtained theoretically with that observed experimentally [8].

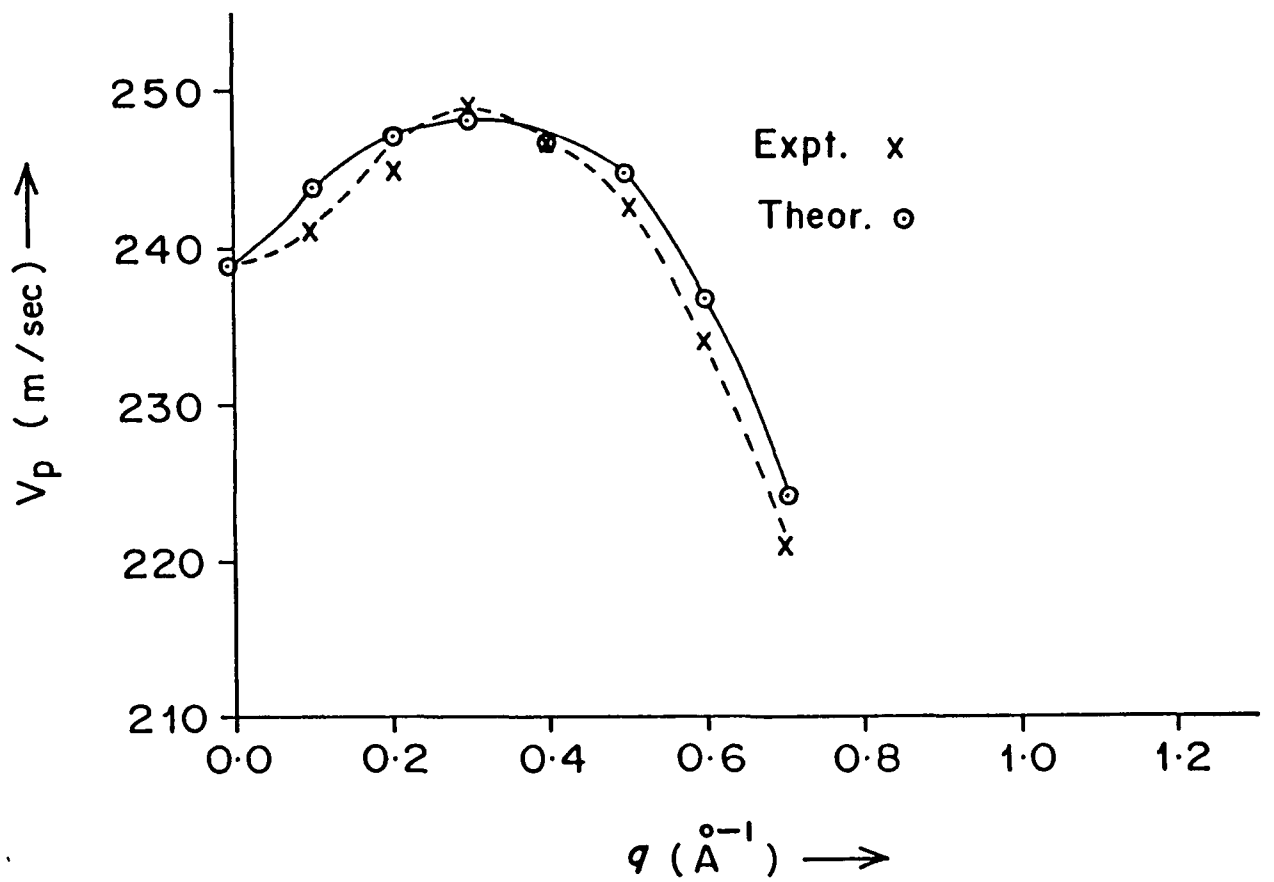


Fig.3.5: Comparison of phase velocity v_p obtained theoretically with that observed experimentally [12].

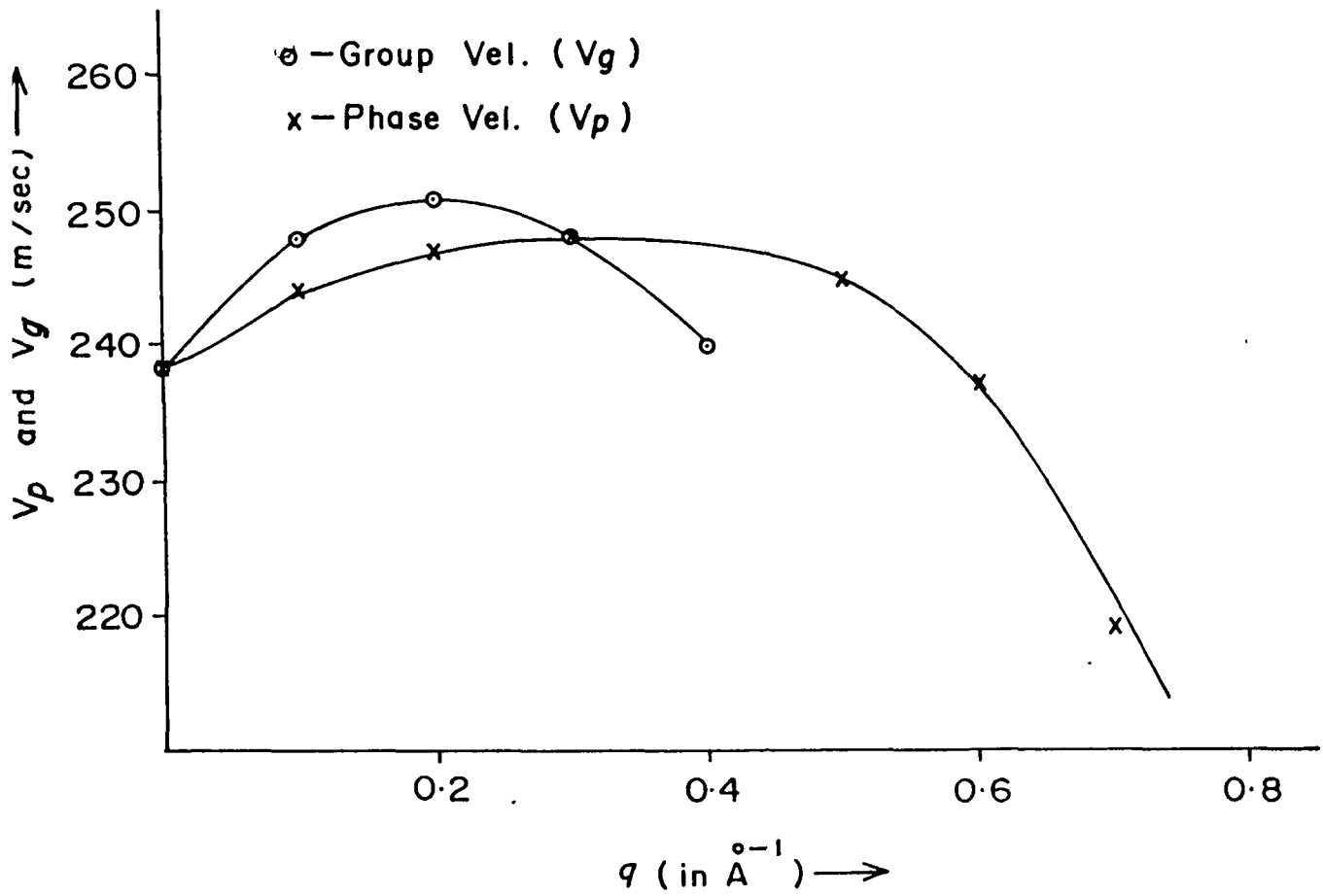


Fig.3.6: Curve of v_p (phase velocity) and v_g (group velocity) obtained theoretically.

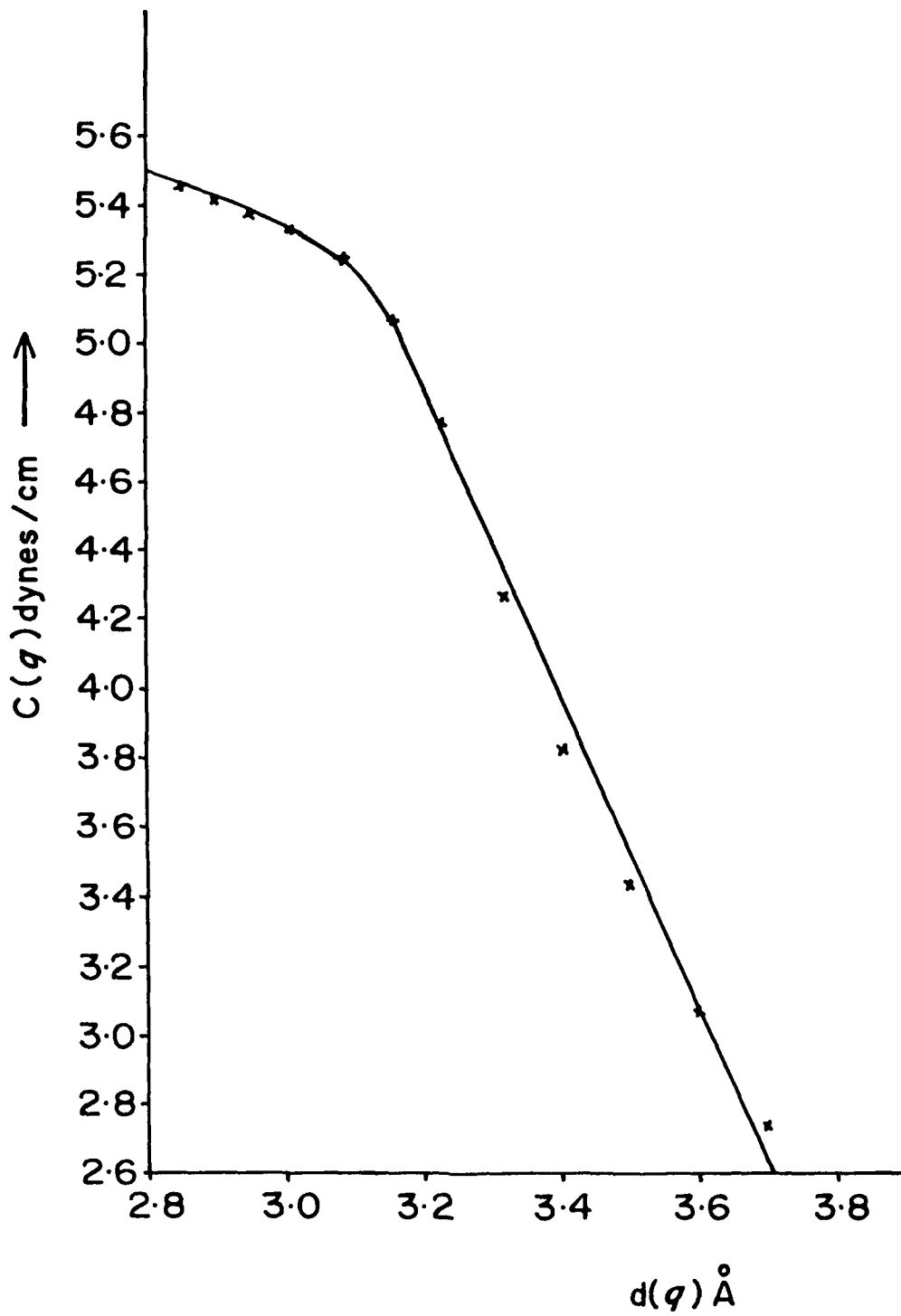


Fig.3.7: Variation $C(q)$ (force constant) with $d(q)$ (interatomic separation).

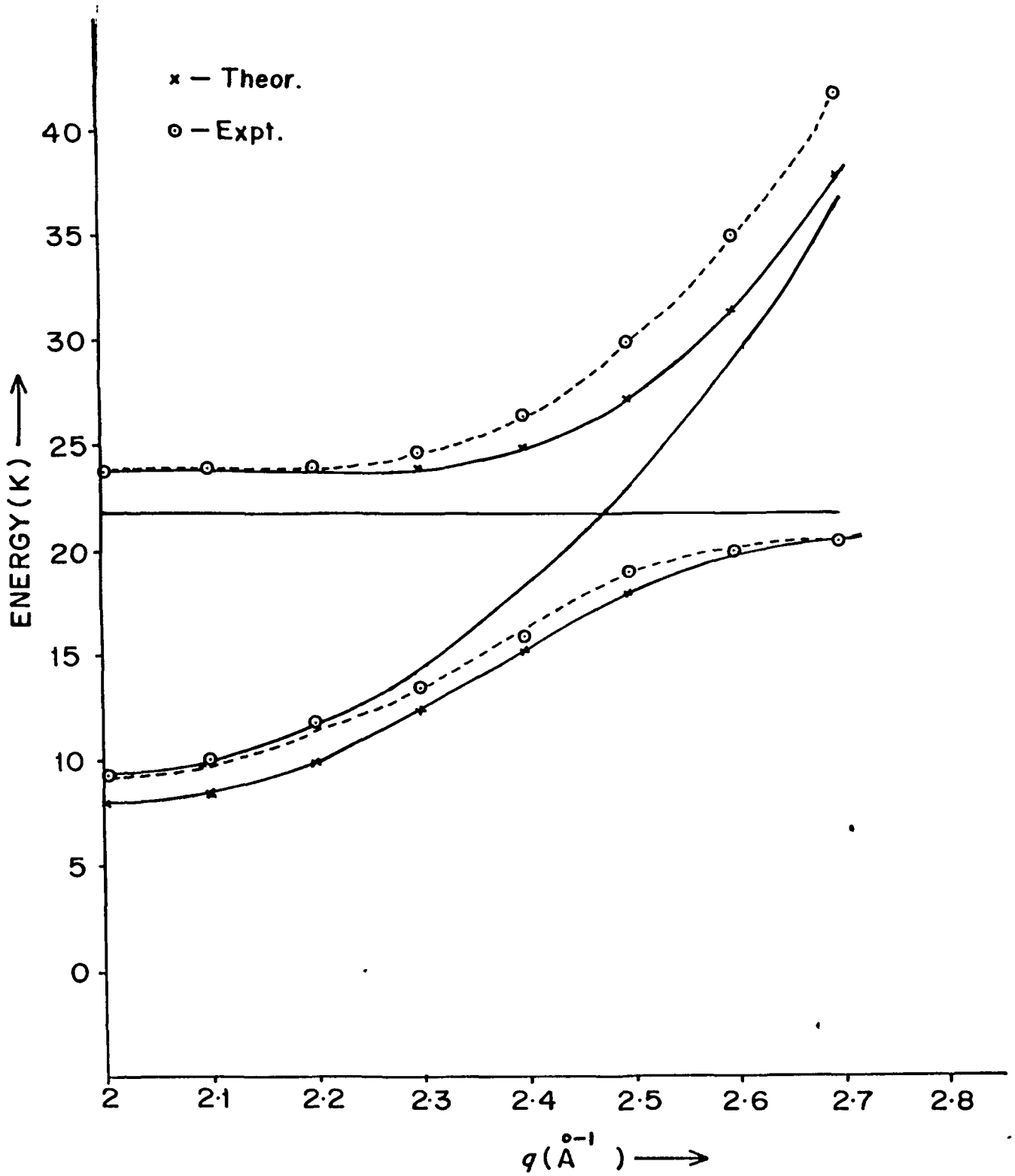


Fig.3.8: Comparison of Theoretically (full line) and Experimentally (dotted line) [19] observed curve of mixing of the single particle excitation and the multiphonon mode.

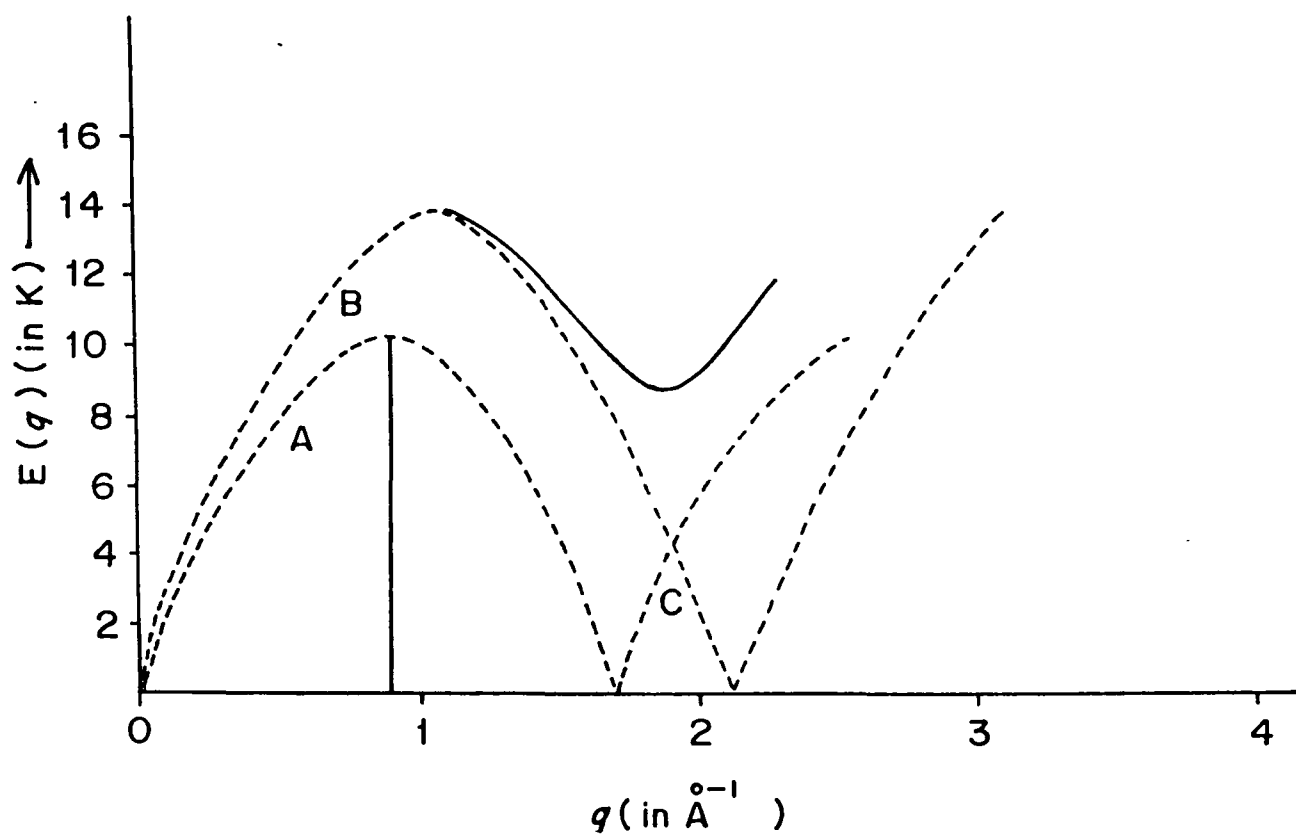


Fig.3.9: Dispersion curve for interatomic separation d and σ

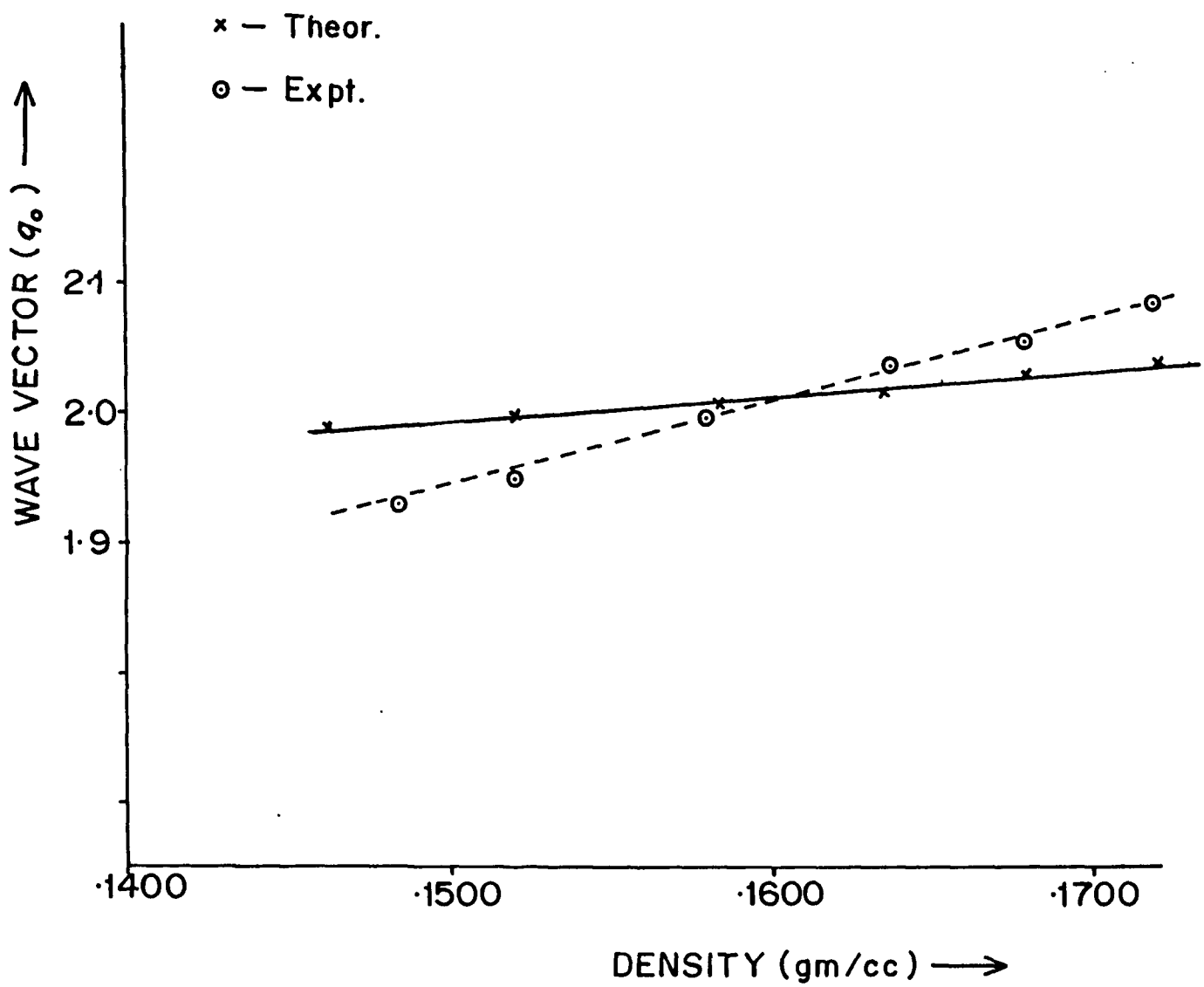


Fig.3.10: Comparison of roton position (q_0) obtained theoretically with that observed experimentally [32].

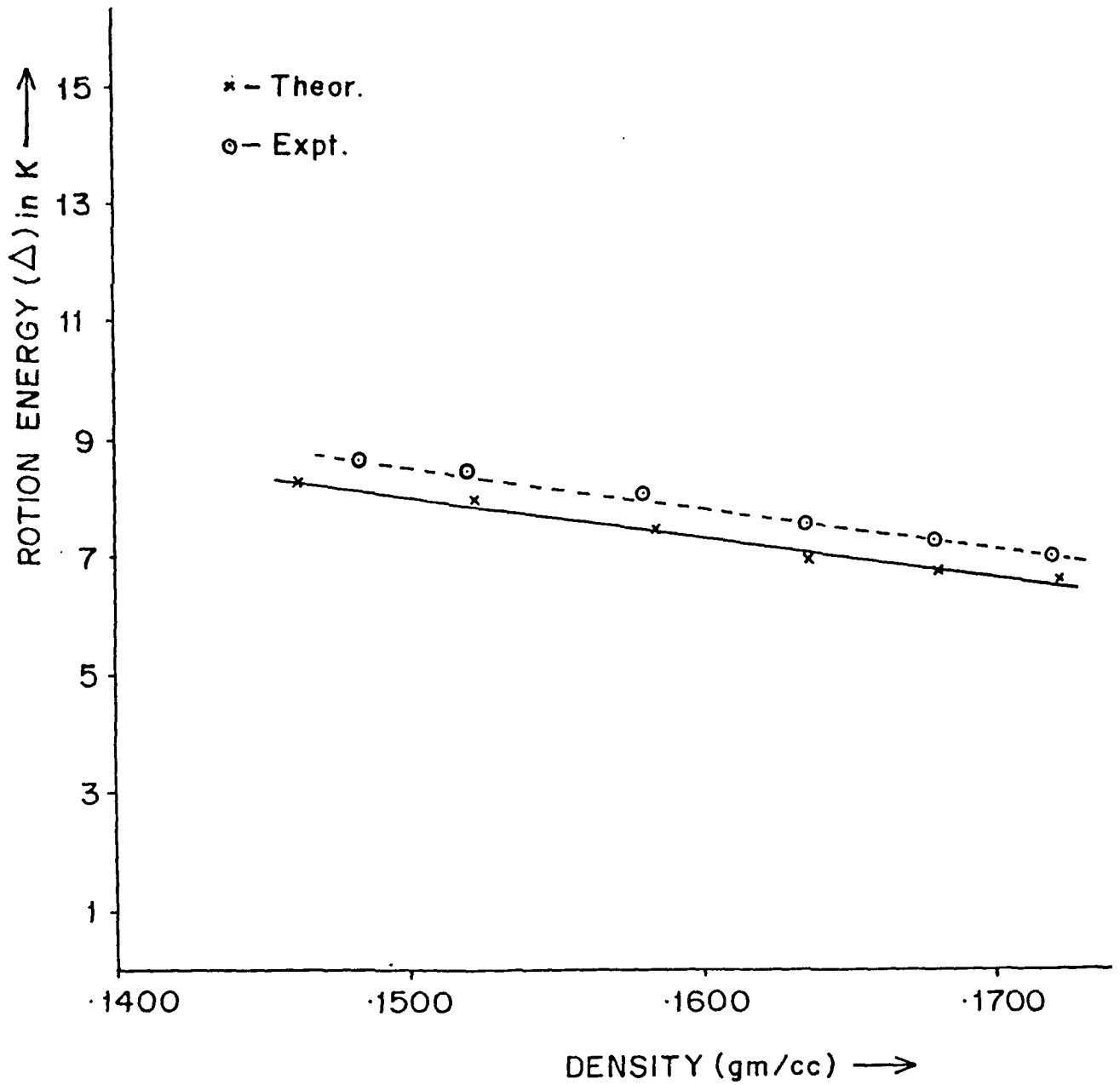


Fig.3.11: Comparison of roton energy (Δ) obtained theoretically with that observed experimentally [33].

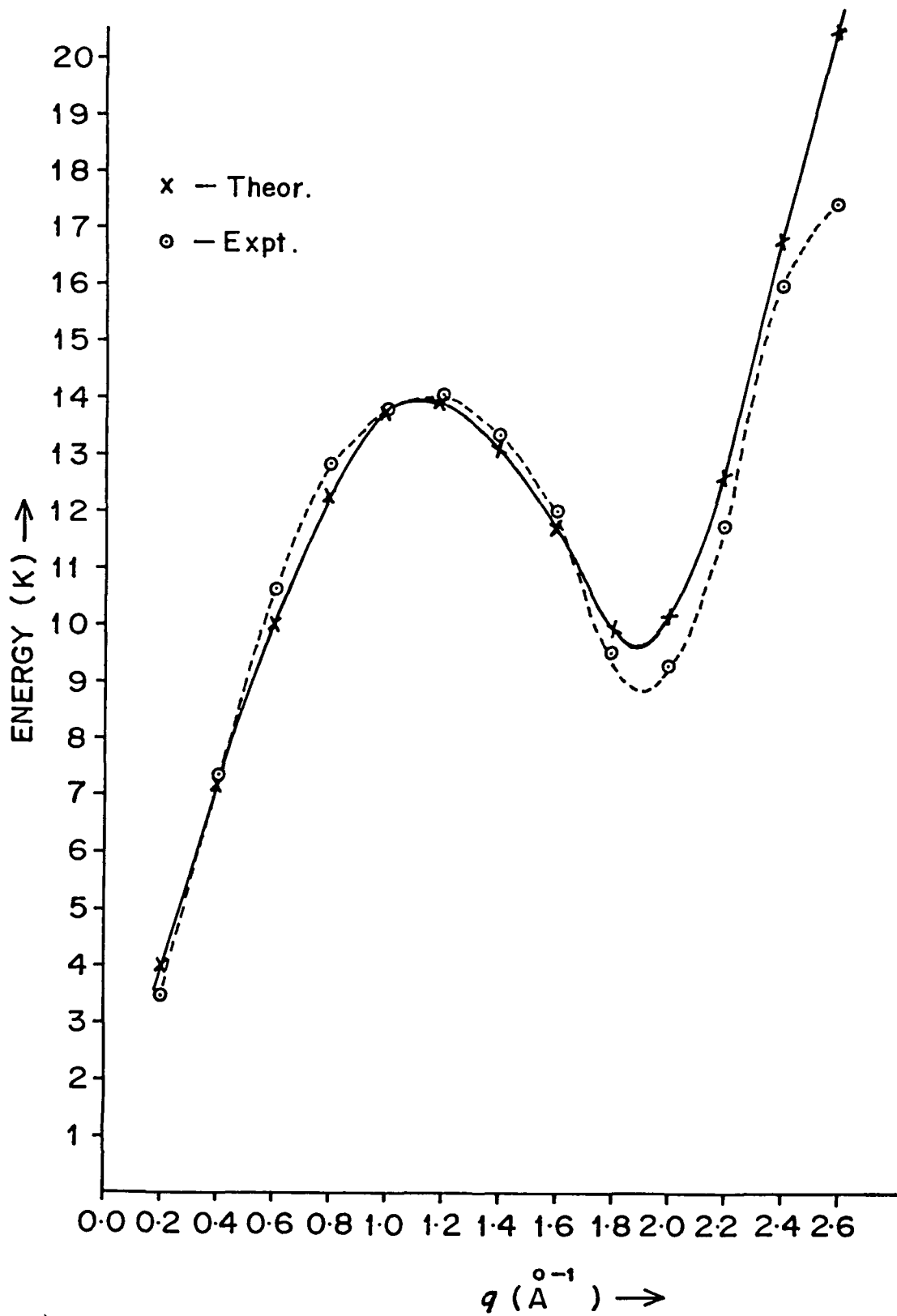


Fig.3.12: Comparison of $E(q)$ obtained through structure factor by replacing m by $2m$ with that observed experimentally [8]

CHAPTER: IV

CALCULATION OF THE VELOCITY
OF THE FIRST, SECOND, THIRD AND FOURTH SOUND

ABSTRACT

Velocity of different sound modes has been studied in detail by using Jain's theory. The temperature dependence of first sound at svp reveals that the configurational arrangement of wavepackets in normal space changes from fcc to sc through bcc as the temperature is lowered through T_{λ} . The pressure dependence of first sound at constant temperature has been analysed to find its relation with pressure by least square fit method. This has also been studied to determine the pressure dependence of interatomic force constant. ρ_s and ρ_n have been obtained at different T from the energy gap and these have been used to find the T dependence of the velocity of second sound. An inter-relationship between v_s , film thickness and the velocity of third sound has been studied to show that the energy gap vanishes at the boundary. The T dependence of the velocity of the fourth sound is also obtained.

4.1 INTRODUCTION

The study of the propagation of sound in many system forms an interesting subject. Normally sound propagate as collective motions of atoms and molecules leading to variation of pressure and density. However, in a system like liquid Helium, we find that at $T \leq T_\lambda$, the system also sustains oscillation of temperature and entropy. This peculiar behaviour was predicted for the first time by London [1] and Tisza [2] and was subsequently shown by Landau [3] through his elegant mathematical theoretical formulations. In this chapter, we use Landau's model to introduce these modes of sound along with the other modes of sound, viz., namely Third and Fourth sounds, known to exist under specific sample conditions. Later we use Jain's model to calculate the velocity of these sounds in He-II and compare such results with experimental values. However, before we proceed to present our investigation, we use two fluid hydrodynamics of Landau to introduce these modes of sound.

Landau [3] used the concept of two fluids to develop an elegant phenomenological theory based on the following relations

$$\rho_n + \rho_s = \rho \quad (1)$$

$$\mathbf{j} = \rho_n \mathbf{v}_n + \rho_s \mathbf{v}_s \quad (2)$$

$$\text{div } \mathbf{j} = -\partial_t / \partial t \quad (3)$$

$$\partial j / \partial t = - \text{grad } P \quad (4)$$

$$\partial(\rho S) / \partial t = - \text{div} (\rho S \mathbf{v}_n) \quad (5)$$

$$\partial \mathbf{v}_s / \partial t = S \text{ grad } T - 1/\rho \text{ grad } P \quad (6)$$

Where

j = the momentum of unit volume of liquid He.

\mathbf{v}_n = velocity of the normal-fluid.

\mathbf{v}_s = velocity of the superfluid component.

S = entropy of the system.

T = temperature of the system.

P = pressure of the system.

Using Equations (1 - 6), one may easily obtain

$$\partial^2 \rho / \partial t^2 = (\partial P / \partial \rho)_S \nabla^2 \rho + (\partial P / \partial S)_\rho \nabla^2 S \quad (7)$$

$$\partial^2 S / \partial t^2 = (\rho_s S^2 / \rho_n) [(\partial T / \partial \rho)_S \nabla^2 \rho + (\partial T / \partial S)_\rho \nabla^2 S] \quad (8)$$

which have solutions of the form

$$\rho = \rho_0 + \rho' \exp [i\omega(t - x/c)] \quad (9)$$

$$S = S_0 + S' \exp [i\omega(t - x/c)] \quad (10)$$

where ω is the angular frequency and c is the velocity.

Using Equations (7 - 10), we have

$$\left\{ \left[\frac{c}{c_1} \right]^2 - 1 \right\} \rho' + \left(\frac{\partial P}{\partial S} \right)_\rho \left(\frac{\partial \rho}{\partial P} \right)_S s' = 0 \quad (11)$$

$$\left(\frac{\partial T}{\partial P} \right)_S \left(\frac{\partial S}{\partial T} \right)_\rho \rho' + \left\{ \left[\frac{c}{c_2} \right]^2 - 1 \right\} s' = 0 \quad (12)$$

$$\text{where } c_1^2 = \left(\frac{\partial P}{\partial \rho} \right)_S \quad (13)$$

$$\text{and } c_2^2 = \left(\frac{\partial S}{\partial T} \right)_\rho \left(\frac{\partial T}{\partial S} \right)_\rho \quad (14)$$

where equation (13) and (14) stands for the velocity of first and second sound.

4.2 FIRST SOUND

As shown in Eqn. 13, the first sound c_1 refers to the propagation oscillations of the normal density at constant entropy. c_1 has been determined under SVP from the wavelength of sound at a known frequency [4] and also by observing the time of flight of a sonic pulse [5]. Accurate measurement at frequencies between 200 and 1450Kc/s using both an accoustical [6,7] and optical interferometer [8,9] have also been carried out. Several other measurements are also reported [10-16].

4.3 SECOND SOUND

The expression for c_2 (Eqn. 14) refers to a wave where the density remains constant. What follows from Eqn. 14, the second sound is the propagation of the oscillations of temperature (or entropy) at constant density. The constant density is maintained by out of phase oscillations of the normal and superfluid components of the system. The second sound is, therefore, observed by similar methods used to measure ordinary sound; the sound generator and detector (i.e microphones) are, however, replaced by a heater and a thermometer. The first observation of this phenomenon was made by Peshkov [17,18]. Similar experiments were made by Lane et. al [19]. The measurement of c_2 gives directly the values ρ_n and ρ_s . The temperature wave present in materials other than He-II do not give rise to standing waves as observed in He-II because of energy dissipation and is not observed. Several other experiment on second sound have been reported thereafter [20-31].

4.4 THIRD SOUND

The existence of third sound and fourth sound was predicted by Atkins [32]. The third sound is a surface wave on He-II film in which the superfluid oscillates parallel to the substrate,

while the normal fluid is clamped because of its viscosity. To a good approximation the phase velocity of third sound, is derived from a relation for the velocity of a surface wave on a shallow classical liquid of depth d ; i.e

$$v_p^2 = \left[(f\lambda/2\pi) + (2\pi T/\rho\lambda) \right] \tanh(2\pi d/\lambda) \quad (15)$$

Here T is the surface tension and f is the force per unit mass due to the Van der Waals attraction of the substrate. It serves as the main restoring force. For long wavelengths the first term is dominant. Further since only the superfluid component participate in the oscillations the third-sound velocity can be written as

$$c_3 = (\rho_s fd/\rho)^{1/2} \quad (16)$$

The third sound is excited by shining the film by infrared beam chopped at desired frequency. The oscillations of film thickness so produced are detected by polarised light technique. A full introduction to third and fourth sound and an account of the earlier experimental work has been reviewed by Atkins and Rudnick [33].

4.5 FOURTH SOUND

The fourth sound is a pressure wave [32] in He-II inside a superleak, where the normal component is immobilised and only the superfluid is in motion. We have,

$$c_4 = \left[(\rho_s/\rho)c_1^2 + (\rho_n/\rho)c_2^2 \right]^{1/2} \quad (17)$$

Shapiro and Rudnick [34] measured the variation of c_4 with temperature by setting up standing waves of fourth sound in an acoustic resonator. The results obtained agree very well with the theoretical results. An acoustic resonator method was used to obtain high precision ($\approx 0.2\%$) simultaneous measurement of first, second and fourth sound velocity over a range of temperature from 1.2K to T_λ in 50 mK steps, and a range of pressures from SVP to the melting curve in steps of 1 bars by Heiserman et al [35].

4.6 CALCULATION OF FIRST SOUND

According to the microscopic model the dispersion due to collective modes can be understood to a good approximation as the dispersion of a linear chain of atoms with uniform separation of d [36]. It was further noted that particles in the system under equilibrium are locked at the relative phase position $\phi = k.r =$

$2s\pi$ and these positions are restored by the quantum correlation potential U_{ij}^s , if they have any displacement in their phase position. For a small displacement $\delta\phi$ from the equilibrium values of ϕ , U_{ij}^s can be written as [37]

$$U_{ij}^s = -k_B T_0 \ln 2 + (1/4) k_B T_0 \delta\phi^2 \quad (18)$$

Considering ϕ_s as the changed phase position of s^{th} atom, the configurational potential V of the chain of atoms can be expressed as

$$V = -Nk_B T_0 \ln 2 + (1/4) k_B T_0 \sum_{s=1}^{N/2} \left[(\phi_s - \phi_{s-1})^2 + (\phi_{s+1} - \phi_s)^2 \right] \quad (19)$$

using the restoring force ($= -\delta V / \delta \phi_s$) for the phase position of the s^{th} atom, the equation of motion for ϕ_s can be written as

$$\ddot{\phi}_s = - (1/2\beta) k_B T_0 \left[2\phi_s - \phi_{s-1} - \phi_{s+1} \right] \quad (20)$$

Here β is the measure of the inertia of motion on ϕ line in the same manner as the mass appears in the motion described by change in r . Defining

$$\phi_s = \phi_0 \cdot \exp [i(qsd - \omega t)] \quad (21)$$

as a kind of wave solution that satisfies the Eqn. (20), we have

$$\omega^2(\mathbf{q}) = \beta^{-1} \cdot (2k_B T_0) \cdot \sin^2(qd/2) \quad (22)$$

Here q is the wavevector of phononlike wave of the change in the phase position of particles that propagate in the system.

Now as $\phi = \mathbf{k} \cdot \mathbf{r}$, one can express $\delta\phi$ as

$$\delta\phi = \delta\mathbf{k} \cdot \mathbf{r} + \mathbf{k} \cdot \delta\mathbf{r} \quad (23)$$

which can be used to consider the situation where such a change in ϕ occurs either due to change in \mathbf{r} with \mathbf{k} constant or due to change in \mathbf{k} with \mathbf{r} constant. In these situations the collective modes of excitations could be understood, respectively, in terms of phonon-like waves describing change in the position of the particles or that of their momentum coordinates. As in the former case we have

$$\delta\phi = \mathbf{k} \cdot \delta\mathbf{r} = (2\pi/d) \cdot (\mathbf{r}_s - \mathbf{r}_{s-1}) \quad (24)$$

The frequency dispersion $\omega(\mathbf{q})$ for waves associated with the displacement of particles from their equilibrium positions is written as

$$\omega(q) = \sqrt{[(8k_B T_0)/m] (\pi/d) \cdot |\sin(qd/2)|} \quad (25)$$

The phase velocity and group velocity of these excitation can be determined by solving for $v_p = \omega/q$ and $v_g = \delta\omega/\delta q$ respectively. For small q limits, we have

$$v_p = v_g = \sqrt{[(2k_B T_0)/m] \pi} = h/\pi/2md \quad (26)$$

The variation of the first sound velocity as a function of temperature is analysed in this section by using Eqn. 26. For this analysis, we assumed three possible structures of the system, viz.: (i) simple cubic ($d = a$) (ii) b.c.c ($d = 1.09a$) (iii) f.c.c ($d = 1.22a$), as well as the mixture of simple cubic and b.c.c with average $d = 1.035a$. The results are given in Table 4.1 and are also depicted in Fig. 4.1 alongwith the experimental results. As such the theoretical and experimental results are in good agreement. However, if we follow the T variation of the experimental values in the direction of decreasing T , we find that our results for fcc arrangement are in better agreement at $T > T_\lambda$. With T decreasing across T the results match with those of bcc arrangement and latter with those of the assumed mixture of sc and bcc. This concludes that the average spatial configuration of the system moves from fcc arrangement to that of the mixture through

bcc arrangement. We note that the experimental curve (cf Fig 4.1) shows a dip at $T = T_c$ contrary to a cusp observed in theoretical curve. The difference could be explained in terms of large fluctuations in the order parameter at $T = T_c$ leading to absorption of sound at this point. Note that Eqn. 26 has been obtained without taking this into consideration.

The value of the first sound is also calculated in this section by applying the above formula as a function of pressure (P) at constant temperature. It may be mentioned that Eqn. (26) gives V_p and V_g which agree well with their experimental values at svp. However, with increasing pressure, the difference in the experimental and theoretical values increases. The reason lies in the following facts:

(i) the pressure may bring certain changes in the atomic arrangement of the system at the microscopic level and d could assume values shorter than that determined by using bcc arrangement.

(ii) the increase in the inter-particle force constant due to increased distortion/polarisation of the ^4He adds additional restoring force to that considered in deriving Eqn. 26 and the

system tend to become more stable.

A least square fit of the pressure dependence of the experimental values of c_1 (for $q \approx 0$) at constant T reveals that

$$c_1 = v_p = v_g = h/\pi/2md + 5p^{1/2} + 3.45p - 0.015p^2 \quad (27)$$

The values of the first sound calculated by applying Eqn. (27) are given in Table 4.2 at T = 1.25, 1.50 and 1.75K, alongwith the experimental data for comparison. As shown in Figs. 4.2 - 4.4, we note that these values agree well with the experimental results.

In order to understand the change in the strength of inter-particle interaction, we examined the variation of the force constant C with P for $q \approx 0$. For this purpose we use

$$C = \frac{v_g^2 m}{d^2 \cos^2(\frac{1}{2} q d)} \quad (28)$$

which has been obtained from the dispersion relation for a single atomic chain (Eqn. 3.2)

The value of d was calculated from the density data [38],

while v_g was taken from the work of Atkins and Stasior [39]. The value of C calculated for different P at constant T are given in Table 4.3. As shown in Figs. 4.5-4.8, the variation of C with P is found to linear.

4.7 CALCULATION OF SECOND SOUND

It follows from Jain's theory that the system below T_λ develops a kind of collective binding that could be defined by an energy gap $E_g(T)$ between the normal and superfluid states of the system. We have

$$E_g(T) = \frac{h^2}{4md_\lambda^3} (d_T - d_\lambda) \quad (29)$$

Once again as suggested by Jain $E_g(T)$ can be used to obtain the superfluid density ρ_s through

$$\rho_s(T) = \frac{E_g(T)}{E_g(0)} \rho \quad (30)$$

and ρ_n through $\rho_n = \rho - \rho_s$. We used the values of $E_g(T)$ obtained by Jain to determine ρ_s and ρ_n tabulated in Table 4.4 (see Figs. 4.9-4.10) alongwith their values determined by Wood and Hollis Halett [40] from the temperature variation of experimental values of c_2 . We find that the two results agree closely.

The following relation for c_2 as a function of temperature was obtained by Peshkov [24]

$$c_2 = \sqrt{\frac{TS_s^2}{C\rho_n}} \quad (31)$$

By using C from the data of Keeson et.al [41] and s from Kapitza's data [42] tabulated in Table 4.5, the value c_2 was calculated as a function of temperature by using our values of ρ_n and ρ_s (cf Table 4.4.). The values of c_2 so obtained are given in Table 4.6 (see Fig 4.11). They agree well with the experimental results except for a small region where our results are slightly higher. On a qualitative basis the origin of this difference may be ascribed to the fact that second sound has appreciable absorption in this temperature range.

4.8 CALCULATION OF THE VELOCITY OF THIRD SOUND

As has been already mentioned, that the energy gap is identified as a vacuum state, where the omon and the phonon pairs are created and annihilated at equal rates when the system is in equilibrium. Since the amplitude of all allowed modes of omons and phonons vanishes at the boundaries of the system, it is evident that E_g vanishes identically. This causes an energy gap gradient near the bounds of the system. We use these observations to analyse the experimental observations on third sound velocity,

given by

$$c_3 = \left[- \frac{3\rho_s}{\rho} \Omega(d) \right] \quad (32)$$

where

c_3 = velocity of third sound

and Ω = Van der Waal potential

To start with, we first studied the Van-der-Waals potential through the equation given below, taking CaF_2 as the substrate, we have

$$\Omega(d) = - \frac{\alpha}{d^3} \quad (33)$$

where Ω = Van der Waal potential

α = material parameter (2.2×10^{-14} ergs cm^3/gm)

d = distance from the surface substrate

The value of $\Omega(d)$ as shown in Table 4.7, have been used in Eqn. 3.2 to calculate ρ_s .

The values of ρ_s thus calculated are plotted against d in Fig. 4.12. This shows that ρ_s vanishes at the surface of the substrate and follows a positive gradient as d increases

establishing that E_g vanishes at such boundary. Further when d becomes equal or greater than ≈ 5 atomic layers (i.e 18\AA), ρ_s attains its maximum possible value. It also vanishes the interface between the fluid and the vapour when the total thickness is about 15 atomic layers. This not only corroborates an independent inference that E_g and ρ_s vanishes at the boundaries [cf chapter II] but it is interesting that the total thickness of the film on the boundaries of which becomes zero is nearly equal to half the coherence length indicating that the coherence length, as expected plays an important role in the properties of thin films.

4.9 CALCULATION OF THE VELOCITY OF FOURTH SOUND

To calculate the velocity of fourth sound , we have applied Eqn. (17). The values of c_1 and c_2 used are shown respectively in Tables 4.8 and 4.6. The other parameters used in this calculation are the total density (ρ), the normal density (ρ_n) and the superfluid density (ρ_s) and these are given in Table 4.4. The fourth sound velocity obtained us by using these data is tabulated in Table 4.9 and depicted by Fig. 4.13. We find that our result agree well with the experimental results obtained from different techniques.

Table 4.1: The variation of the first sound velocity with temperature

Temp (K)	vel (sc) (m/sec)	vel (bcc) (m/sec)	vel (fcc) (m/sec)	vel (sc +bcc) (m/sec)	vel [*] Expt. (m/sec)
0.2	246.92	226.31	219.96	238.56	237
0.4	246.92	226.31	219.96	238.56	237
0.6	246.92	226.31	219.96	238.56	237
0.8	246.92	226.31	219.96	238.56	237
1.0	246.92	226.31	219.96	238.56	237
1.2	246.92	226.31	219.96	238.56	237
1.4	246.92	226.31	219.96	238.56	236
1.6	246.96	226.36	220.02	238.61	234
1.8	247.07	226.46	220.12	238.72	232
2.0	246.92	226.62	220.27	238.88	227
2.2	246.92	226.83	220.47	239.10	219
2.4	246.92	226.46	220.12	238.72	221
2.6	246.92	225.89	219.56	238.12	221
2.8	246.92	224.32	218.90	237.40	220
3.0	246.92	224.31	218.03	236.45	218
3.2	246.92	223.25	216.99	235.33	215
3.4	246.92	222.02	215.79	234.03	210
3.6	246.92	220.60	214.42	232.53	204

* see Ref. 39

Table 4.2: Velocity of first sound as a function of pressure at constant temperature

Temp. (K)	pressure (atm.)	first sound velocity	
		expt.* (m/sec)	theo. (m/sec)
1.25	5	273	278.99
	10	300	303.11
	15	326	324.79
	20	346	344.75
	25	365	363.36

1.50	5	272	279.10
	10	299	303.17
	15	325	324.89
	20	345	344.96
	25	362	363.61

1.75	5	270	279.21
	10	298	303.43
	15	323	325.26
	20	342	345.42
	25	355	364.31

* see Ref. 39

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Table 4.3: Variation of force constant (C) with pressure (P)

Temp (K)	press. P atm.	velocity v_g^* m/sec	inter-atomic dist. d^{**} Å	force-constant C dyne/cm
1.25	5	273	3.521398	3.994433
	10	300	3.474841	4.953734
	15	326	3.437629	5.976920
	20	346	3.406676	6.855683
1.50	5	272	3.519857	3.968696
	10	299	3.474110	4.922835
	15	325	3.436229	5.945149
	20	345	3.403978	6.826921
1.75	5	270	3.518319	3.913968
	10	298	3.470465	4.900240
	15	323	3.431348	5.888921
	20	342	3.397939	6.732575
1.80	5	269	3.517551	3.886726
	10	297	3.469011	4.871488
	15	321	3.429958	5.820932
	20	339	3.392607	6.635788

* see Ref. 39

** see Ref. 38

Table 4.4: Total, normal and superfluid density of He-II as a function of temperature

temp. (K)	den ($\rho_n \times 10^3$) gm/cm ³ Theor.	den ($\rho_s \times 10^3$) gm/cm ³ Theor.	den ($\rho \times 10^3$) gm/cm ³ Expt.*	den ($\rho \times 10^3$) gm/cm ³ Expt.*
0.2	0.000055	144.9999		
0.3	0.000315	144.9996		
0.4	0.000858	144.9991		
0.5	0.002580	144.9974		
0.6	0.007751	144.9922	0.006191	144.99
0.7	0.022000	144.9780	0.03654	144.96
0.8	0.046000	144.9540	0.14007	144.86
0.9	0.108000	144.8920	0.42775	144.57
1.0	0.247000	144.7530	1.0904	143.91
1.1	0.550000	144.4500	2.262	142.74
1.2	1.373000	143.6270	4.234	140.77
1.3	3.003000	141.9970	6.931	138.07
1.4	5.884000	139.1160	10.933	134.07
1.5	10.604	134.4960	15.95	129.15
1.6	17.832	127.2680	24.65	120.45
1.7	28.305	116.8950	34.8	110.40
1.8	42.807	102.4930	46.4	98.90
1.9	62.170	83.2300	62.35	83.05
2.0	87.20	58.4000	81.2	64.40
2.1	118.696	27.1040	107.3	38.50

* see Ref. 40

Table 4.5: Values of specific heat and entropy as a function of temperature

Temp. (K)	Specific Heat [*] $\text{J.g}^{-1}.\text{deg}^{-1}$	Entropy ^{**} $\text{J.g}^{-1}.\text{deg}^{-1}$
0.2	0.0002	0.00005
0.3	0.0005	0.00018
0.4	0.0013	0.00044
0.5	0.0025	0.00085
0.6	0.0044	0.00147
0.7	0.0098	0.00276
0.8	0.0222	0.00475
0.9	0.0510	0.00885
1.0	0.1042	0.01680
1.1	0.1910	0.01680
1.2	0.3220	0.03040
1.3	0.5160	0.05230
1.4	0.7800	0.08530
1.5	1.1270	0.13200
1.6	1.5720	0.19700
1.7	2.1100	0.28400
1.8	2.8100	0.39500
1.9	3.7900	0.53500
2.0	5.1800	0.71500
2.1	7.5100	0.94000

* see Ref. 41

** see Ref. 42

Table 4.6: Values of second sound as a function of temperature

temp. (K)	second sound (theor.) (m/sec)	second sound (expt) [*] (m/sec)
0.2	120.415	
0.3	118.718	
0.4	107.316	
0.5	102.353	
0.6	074.244	83
0.7	059.880	46.5
0.8	050.617	29
0.9	043.061	21.6
1.0	039.842	18.9
1.1	037.387	18.3
1.2	032.653	18.4
1.3	029.441	19.1
1.4	027.192	19.7
1.5	025.596	20.1
1.6	024.205	20.3
1.7	022.784	19.9
1.8	020.952	18.7
1.9	018.523	16.4
2.0	015.116	12.2
2.1	009.908	

* see Ref. 24

Table 4.7: Value of density of superfluid (ρ_s) from the velocity of third sound (c_3)

distance (atomic layer)	$\Omega(d)$	c_3	ρ_s
1	-4.7×10^8	8000	0.006560
3	-1.7×10^7	5000	0.069188
5	-3772290	3300	0.139530
7	-137441	2000	0.140632
9	-646826	1360	0.138209
11	-354272	1000	0.136429
13	-214627	650	0.095145
15	-139714	400	0.055350

Table 4.8: Values of the first sound as a function of temperature

Temp. (K)	vel. first sound (theor.) (m/sec)	vel. first sound (expt.) [*] (m/sec)
0.2	246.92	238
0.3	246.92	238
0.4	246.92	238
0.5	246.92	238
0.6	246.92	238
0.7	246.92	238
0.8	246.92	238
0.9	246.92	238
1.0	246.92	238
1.1	246.92	237.5
1.2	246.92	237
1.3	246.92	236.5
1.4	246.92	236
1.5	246.97	235
1.6	246.97	234
1.7	247.03	233
1.8	247.09	232
1.9	247.15	229
2.0	247.26	227
2.1	247.37	222

* see Ref. 39

Table 4.9: Values of fourth sound as a function of temperature

Temp. (K)	vel. fourth sound (theor.) (m/sec)	vel. fourth sound (expt.) [*] (m/sec)
0.2	246.92	237.92
0.3	246.92	237.92
0.4	246.92	237.92
0.5	246.92	237.92
0.6	246.91	237.93
0.7	246.90	237.92
0.8	246.88	237.84
0.9	246.83	237.59
1.0	246.71	237.02
1.1	246.46	235.62
1.2	245.77	233.40
1.3	244.38	230.34
1.4	241.92	226.26
1.5	237.88	220.39
1.6	231.46	212.97
1.7	221.88	203.41
1.8	207.83	190.00
1.9	187.38	169.80
2.0	157.03	136.55
2.1	107.03	045.86

* see Ref. 29 and 39

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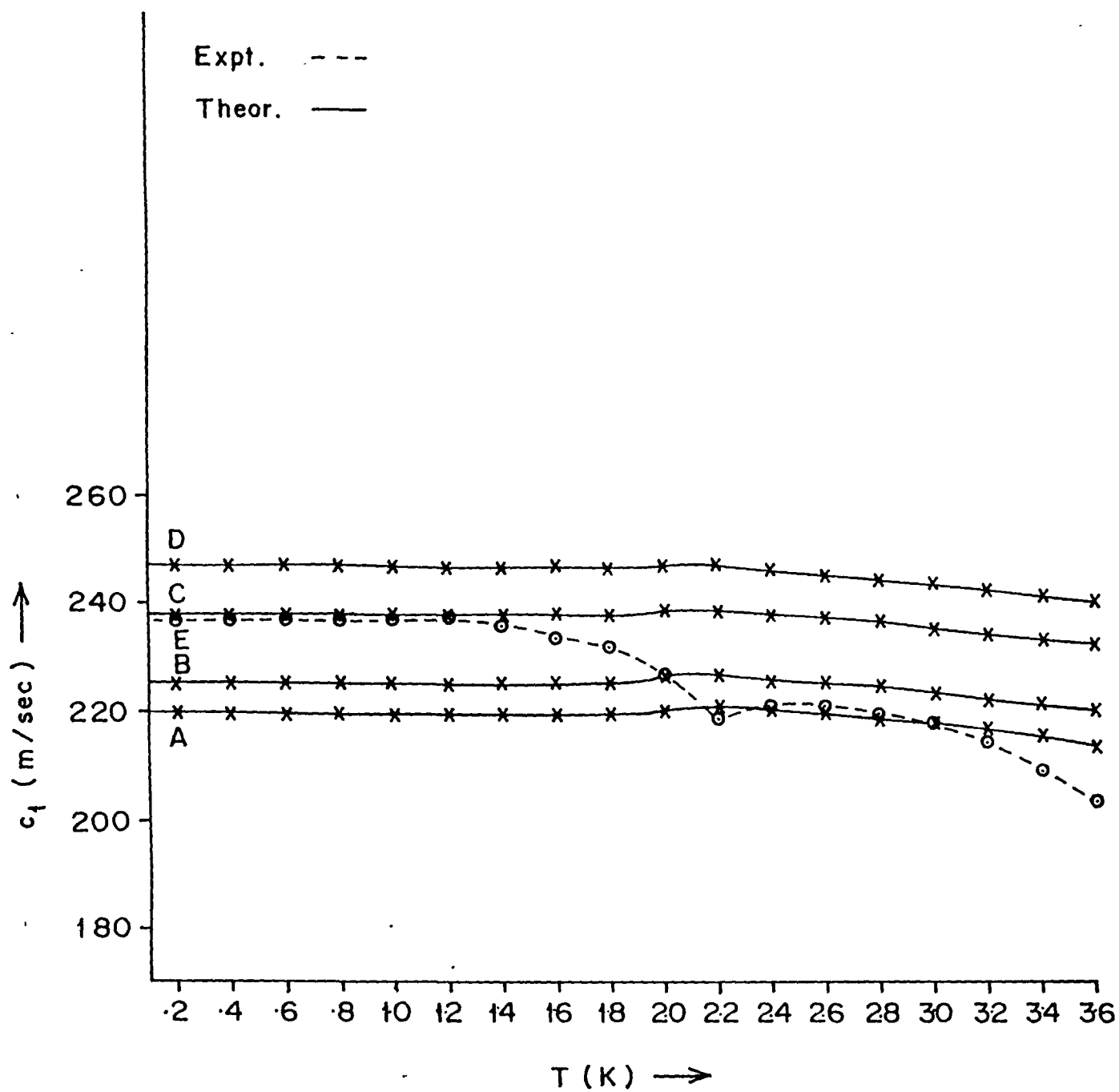
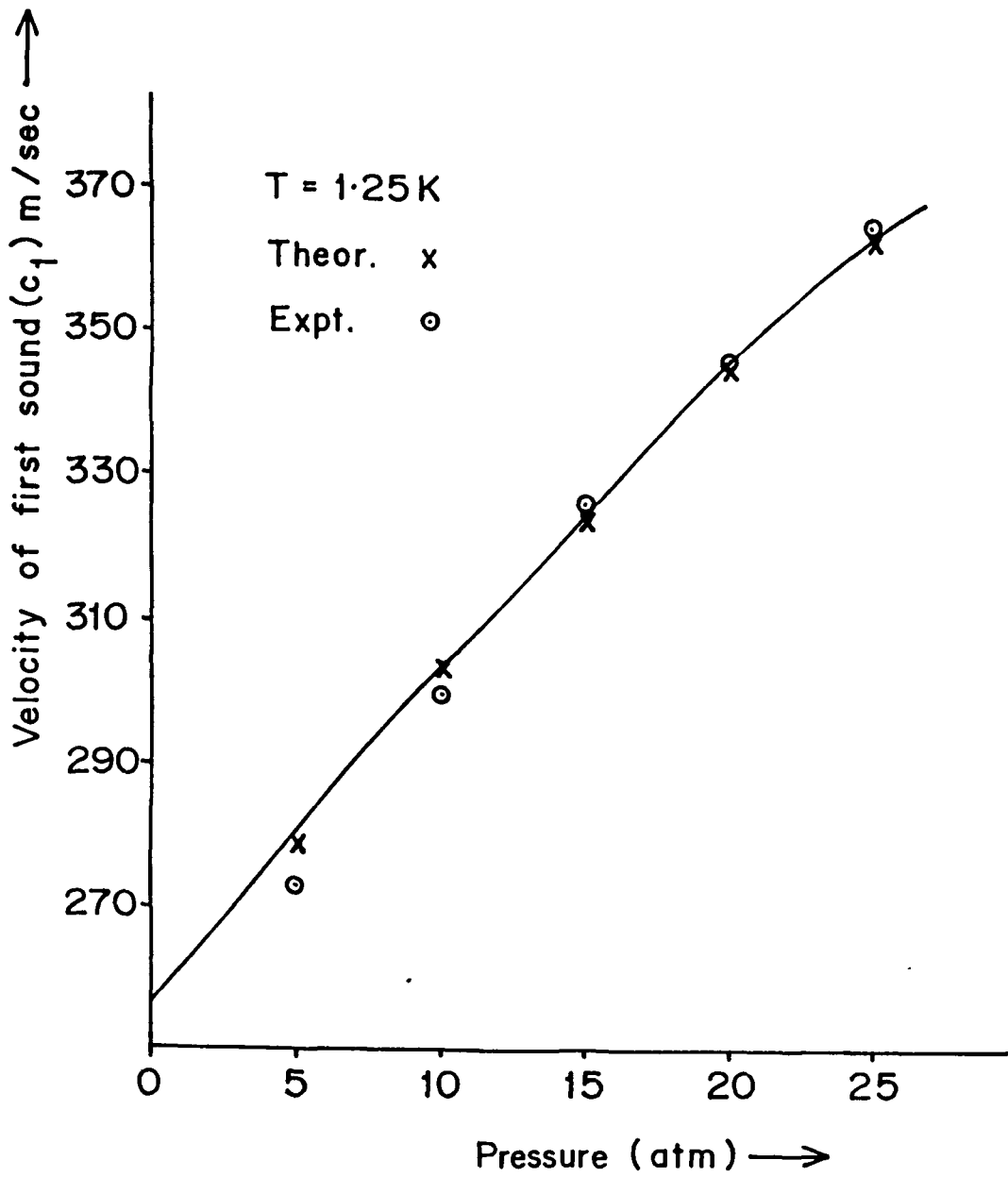


Fig.4.1: Variation of first sound (c_1) as a function of temperature T for four possible structure (A) fcc (B) bcc (C) mixture of sc and bcc (D) sc. (E) Experimentally observed curve (dotted line) [39]



g. 4.2: Variation of first sound (c_1) with pressure at $T = 1.25\text{K}$. The experimental values are shown by dots [39]

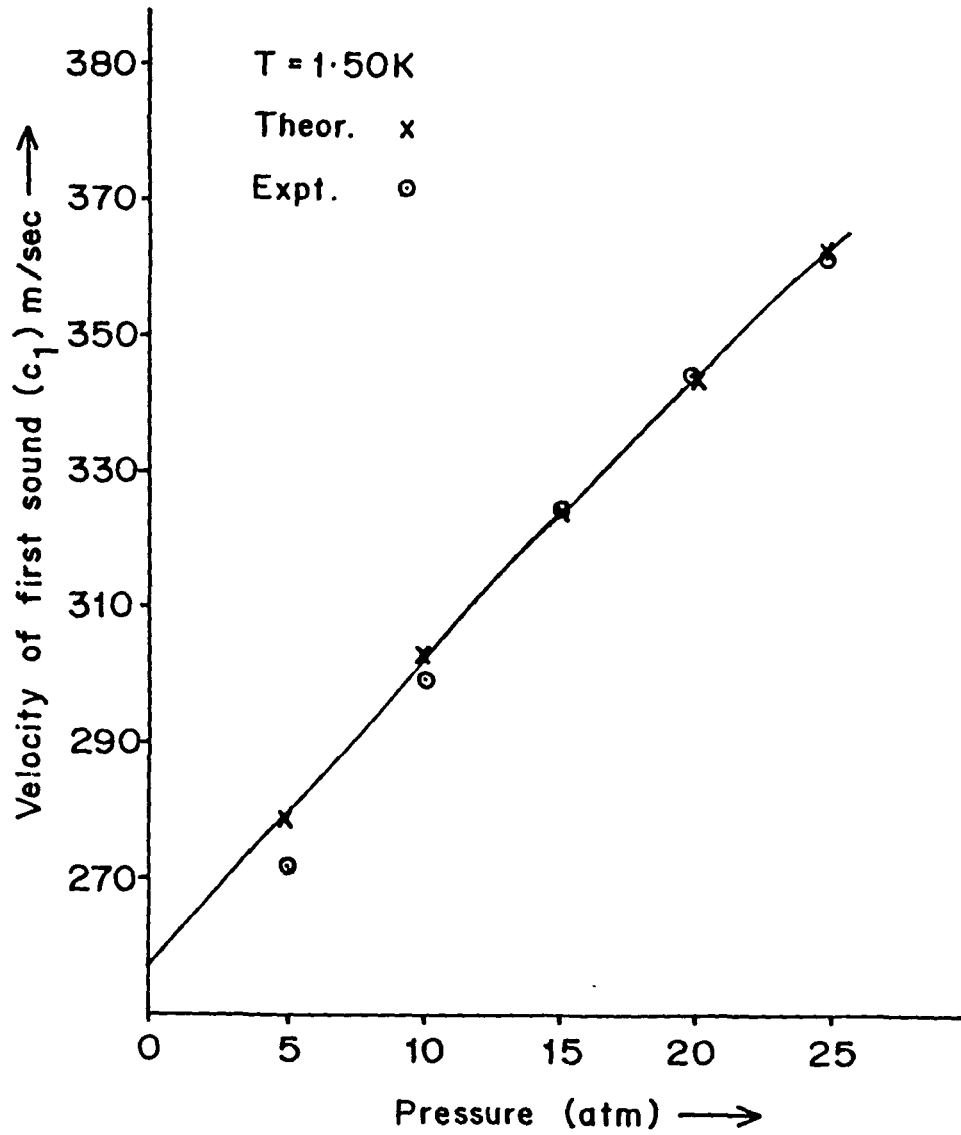


Fig. 4.3: Variation of first sound (c_1) with pressure at $T = 1.50K$. The experimental values are shown by dots [39]

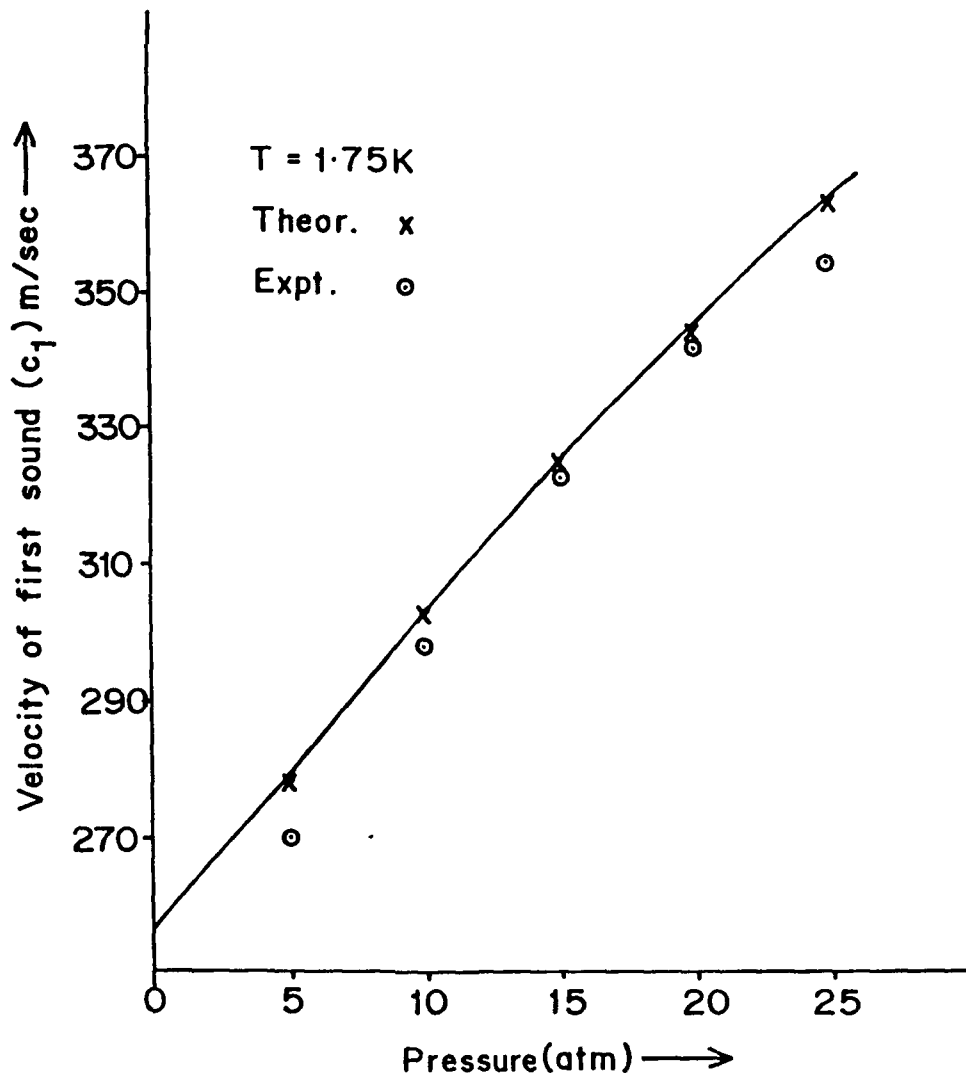


Fig. 4.4: Variation of first sound (c_1) with pressure at $T = 1.75K$. The experimental values are shown by dots [39]

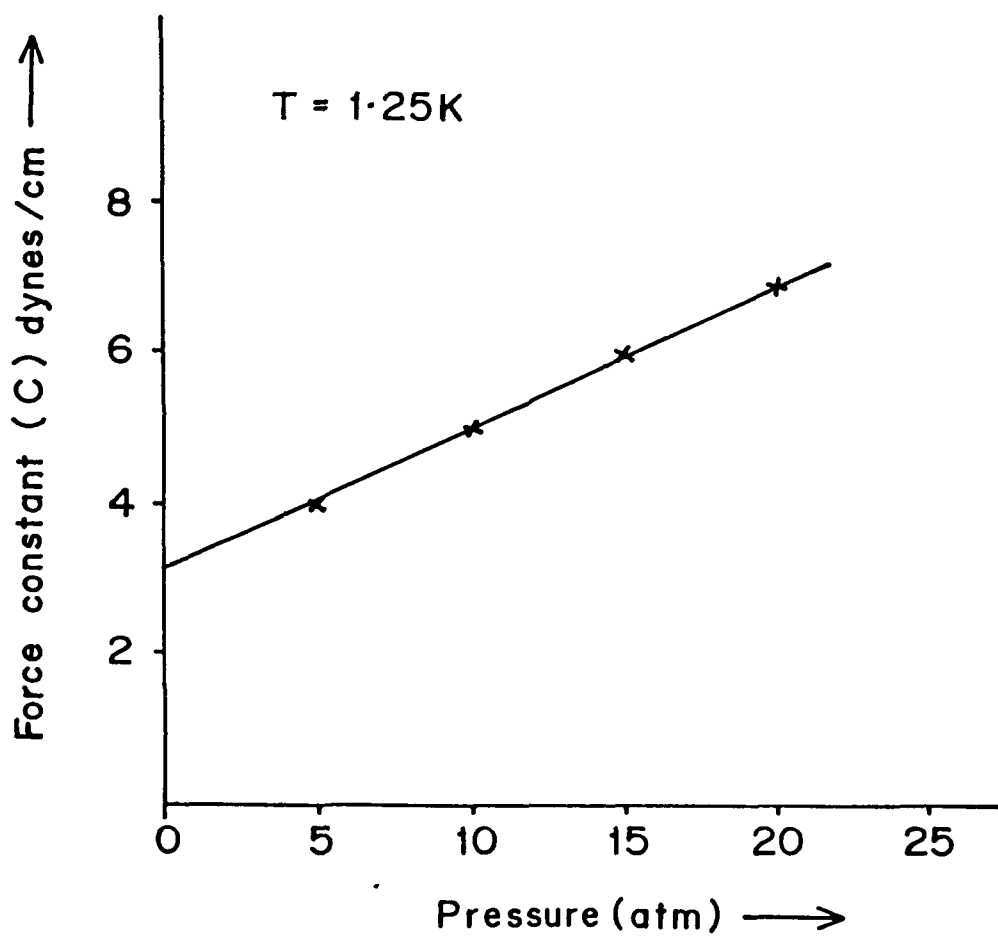


Fig. 4.5: Variation of force constant (C) with pressure at $T = 1.25\text{K}$

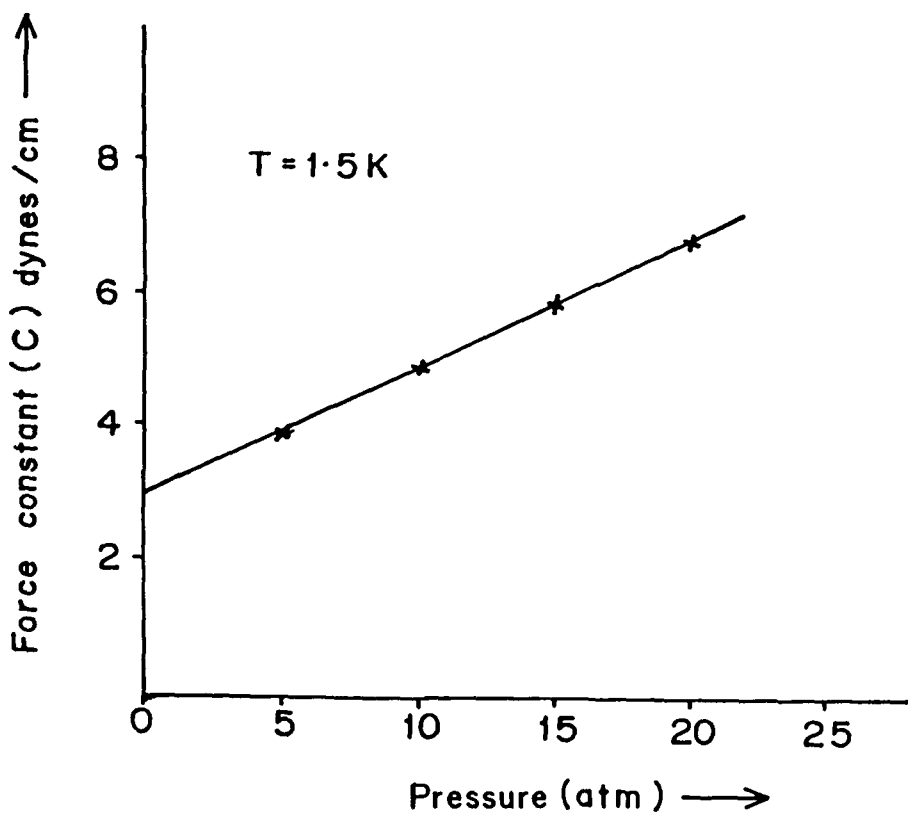


Fig. 4.6: Variation of force constant (C) with pressure at $T = 1.5K$

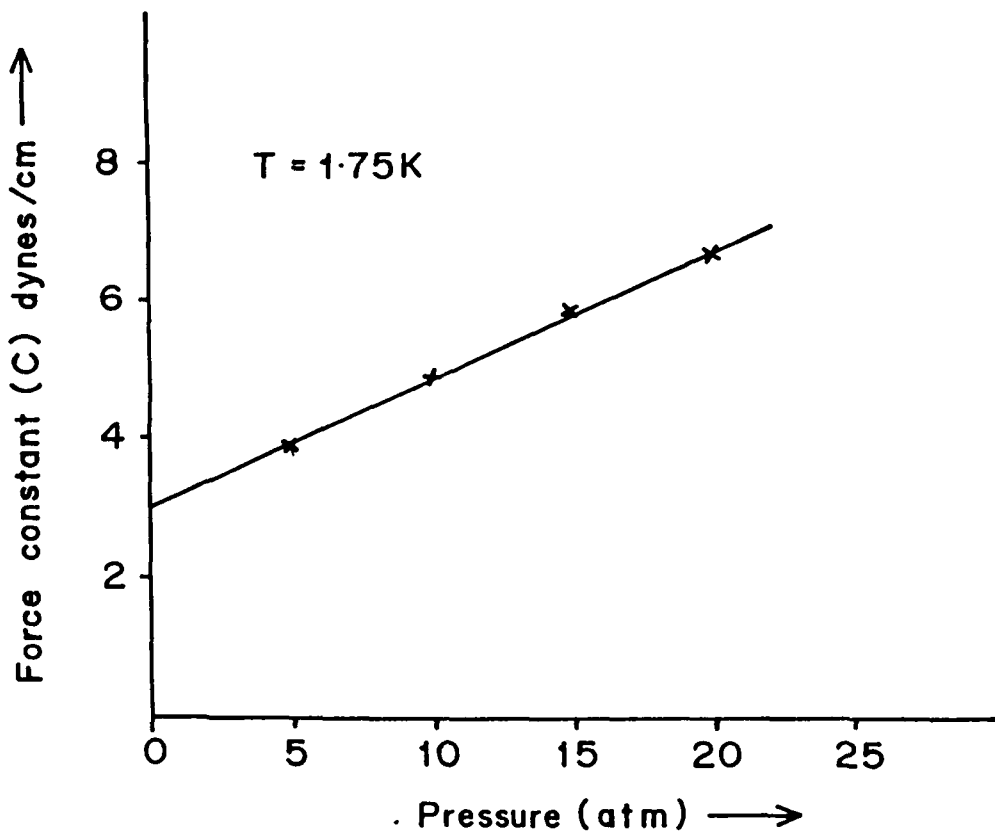


Fig. 4.7: Variation of force constant (C) with pressure at $T = 1.75K$

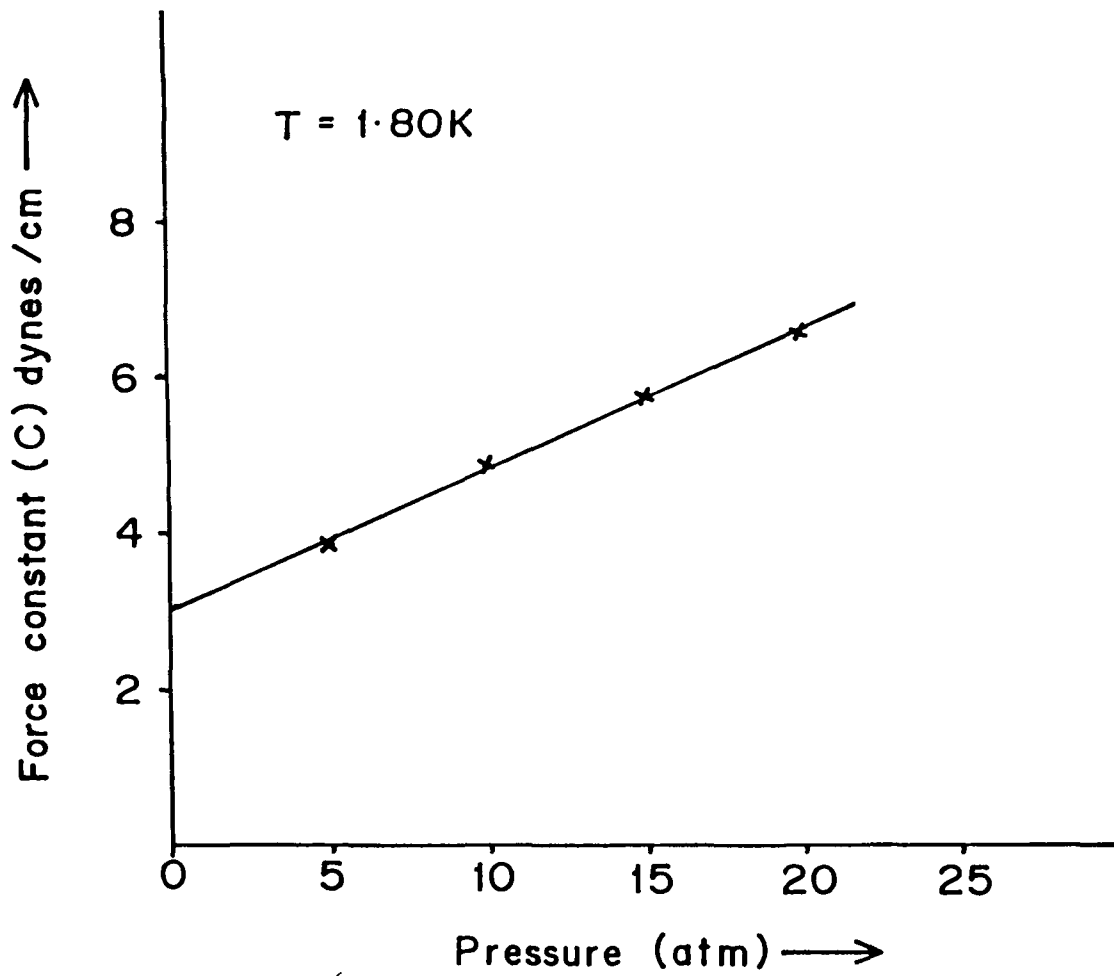


Fig. 4.8: Variation of force constant (C) with pressure at $T = 1.8\text{K}$

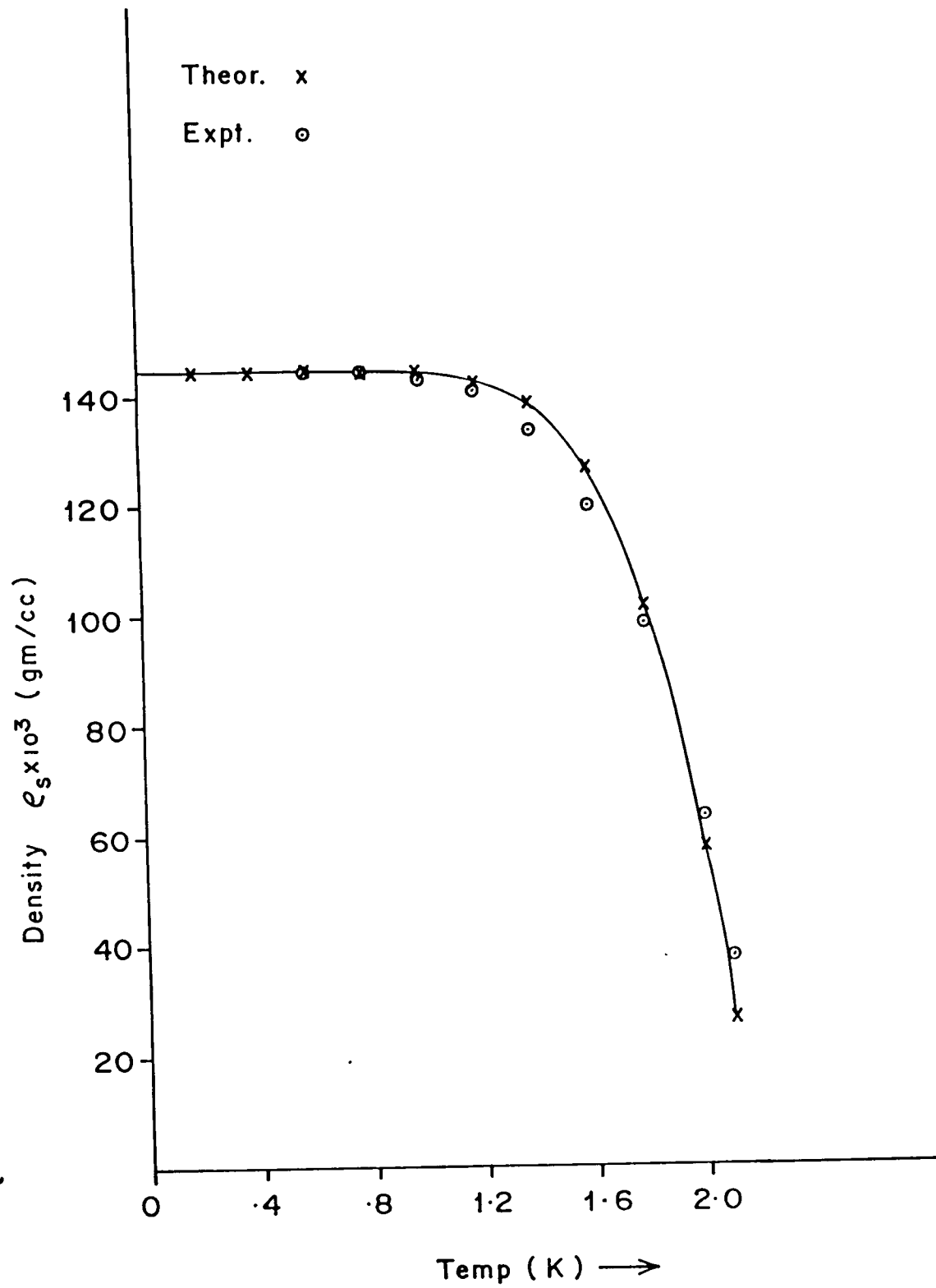


Fig. 4.9: Variation of superfluid density (ρ_s) with temperature T.

The experimental values are shown by dots [40]

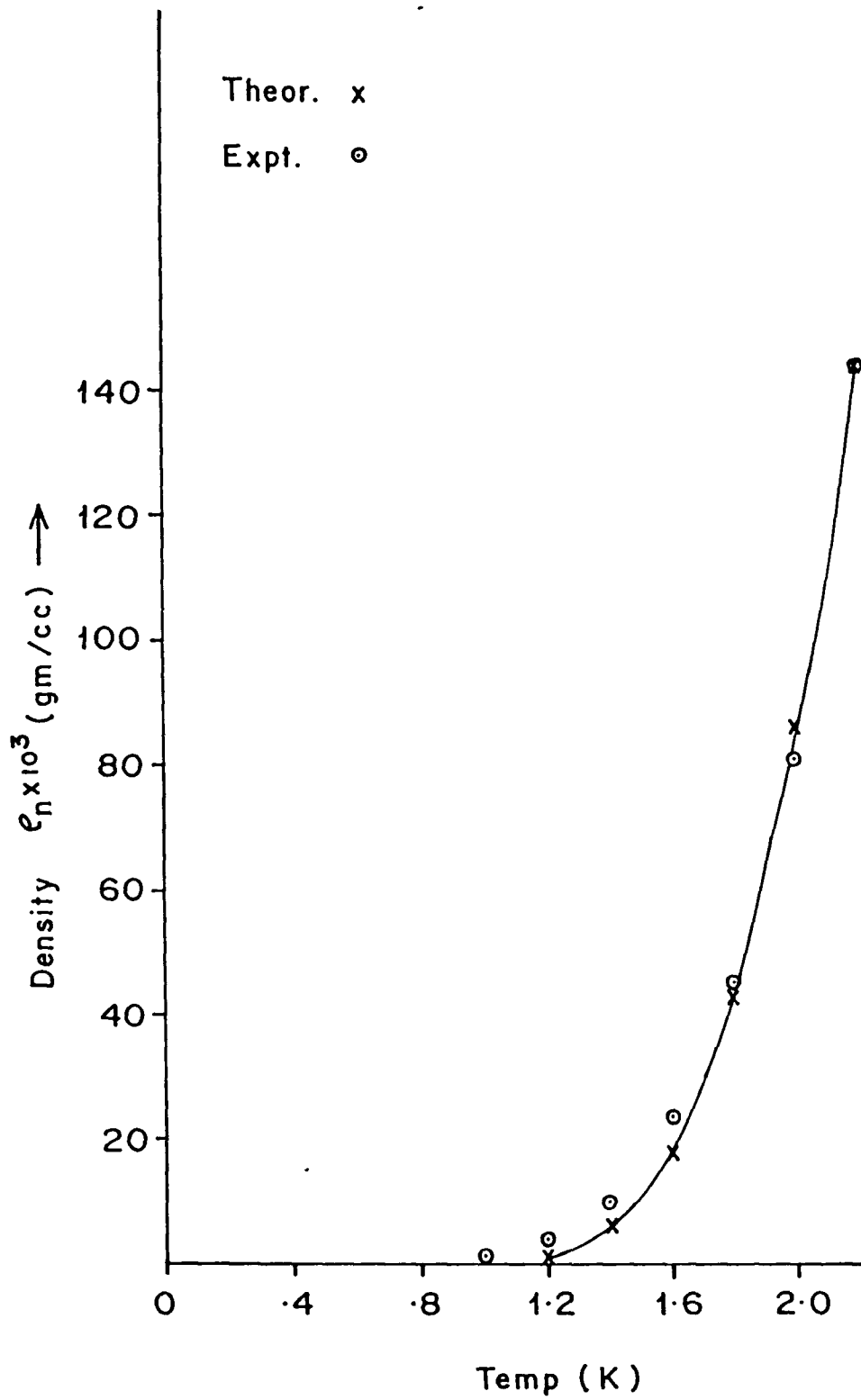


Fig. 4.10: Variation of normal density (ρ_n) with temperature T.

The experimental values are shown by dots [40]

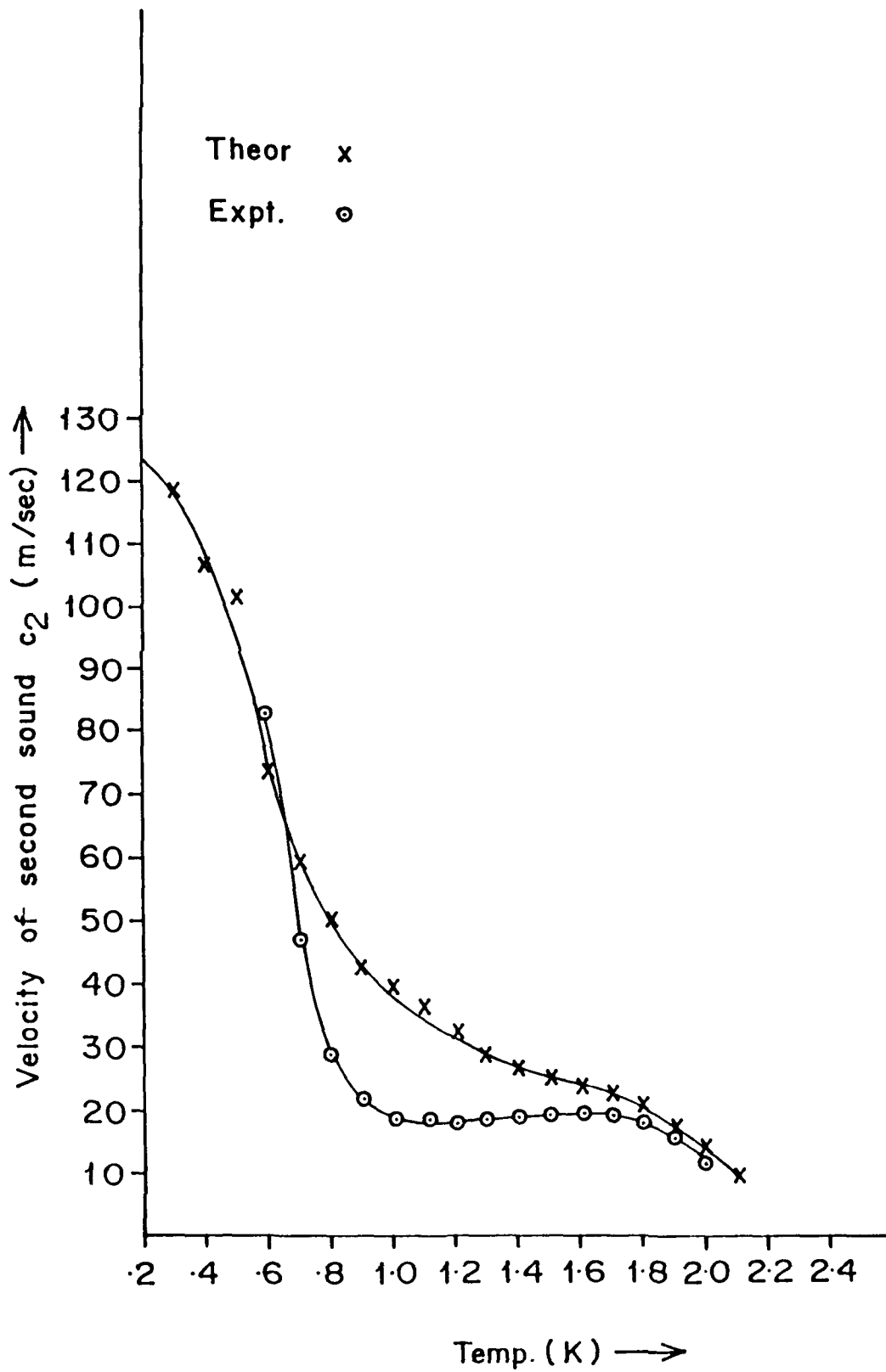


Fig. 4.11: Variation of superfluid density (ρ_s) with temperature T .

The dotted line shows the experimentally observed curve

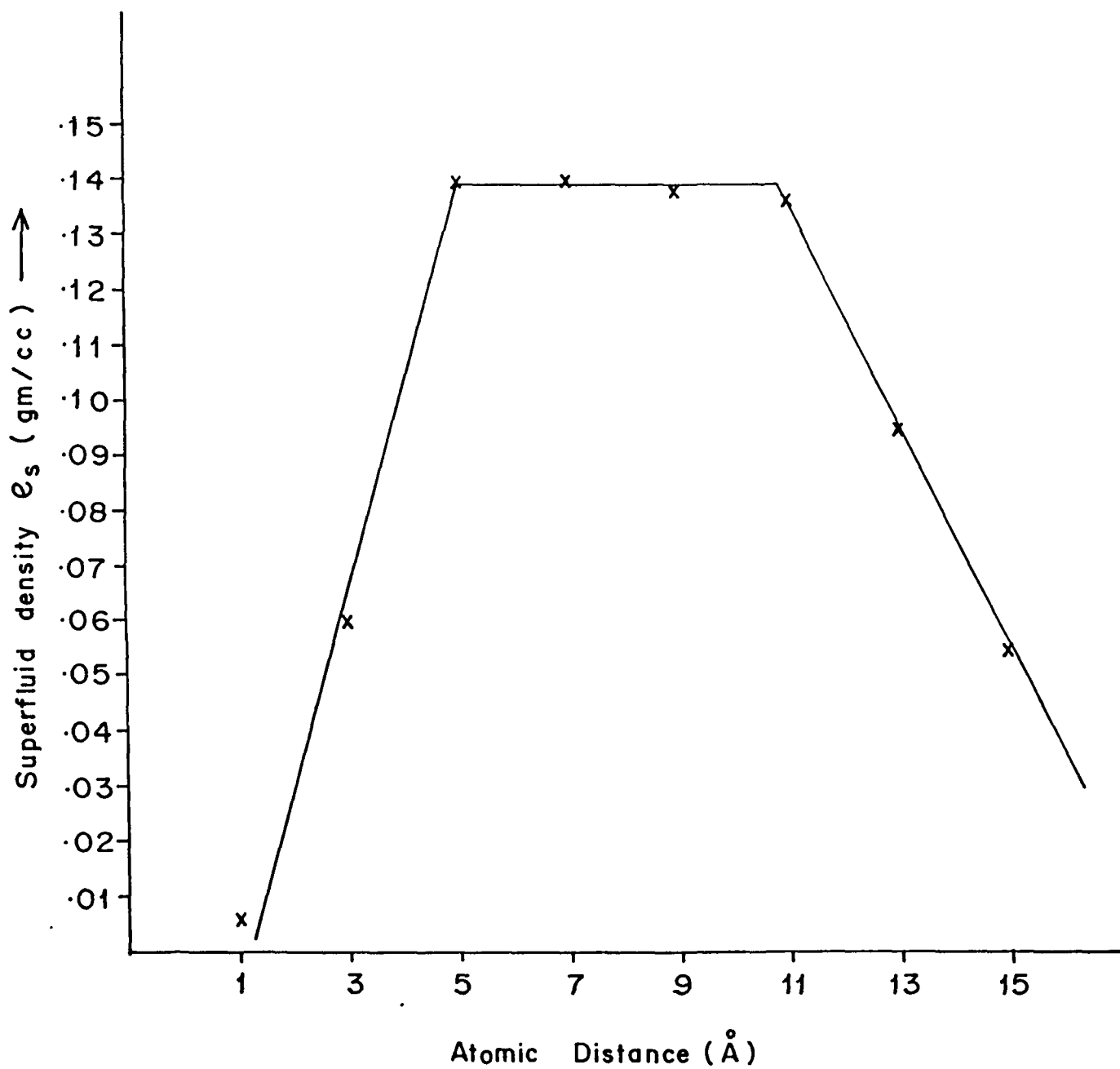


Fig. 4.12: Variation of ρ_s with distance d

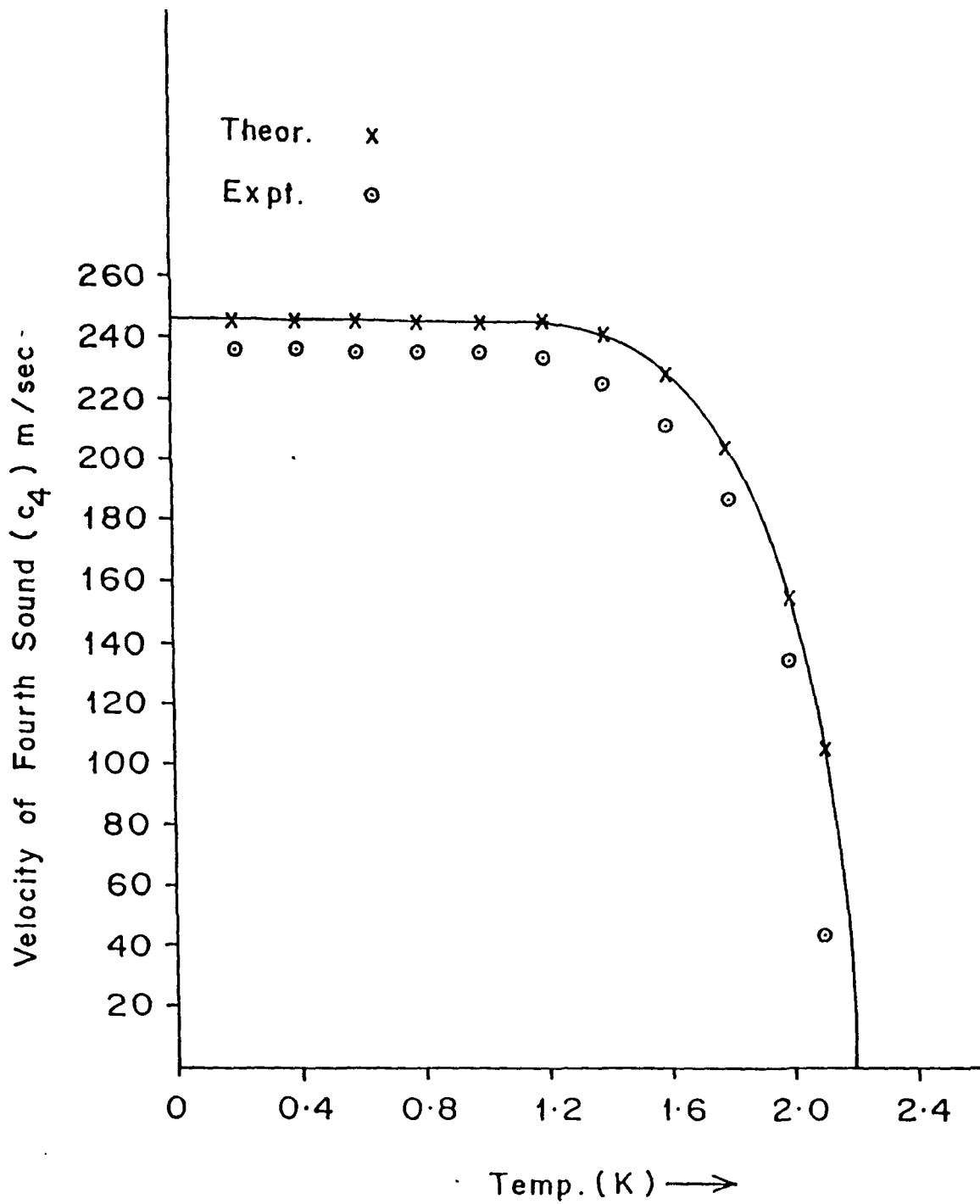


Fig. 4.13: Variation of fourth sound c_4 with temperature T. The dotted line shows the experimentally observed curve [29,30]

CHAPTER: V

RAMAN SCATTERING STUDIES

OF HELIUM-4

ABSTRACT

Summarizing the important observations of experimental and theoretical studies on Raman Scattering of He-II, we present here a new understanding of the origins of different Raman bands. We find that the two maxon mode appears as a weak shoulder in addition to the two roton peak. The unexplained P_3 peak in the high resolution spectrum originates from the two roton mode in the non-interacting configuration. The so called four roton peak seems to arise from the two plateau modes. It is suggested that Raman Scattering needs to be reformulated in the framework of the information of the ground state configuration as rendered by Jain's microscopic theory.

5.1 INTRODUCTION

The Raman scattering (RS) of ^4He was studied only after a theoretical work by Halley [1]. However, the RS studies were summed up as back as in 1976 by Stephen [2], and in 1978 by Greytak [3]. Since then several research papers [4-10] have been published reporting newer information and explanation. A critical review of all these studies on RS reveals that the results are still not understood accurately. Further since the analysis reported in the published work from other laboratories uses different microscopic models which do not agree with recently developed picture of the system revealed from Jain's theory, a systematic analysis using the this model is highly desirable. In this chapter we report such an analysis and its inferences.

5.2 EXPERIMENTAL WORKS ON RAMAN SCATTERING OF HE-II

The intensity and polarization of RS from rotons and higher energy excitations were measured for the first time by Greytak and Yan [11]. In a subsequent paper, Woerner and Greytak [12], reported a high resolution Raman spectrum of the roton region at 1.2 K. Such spectrum of He-II at 0.6K under svp was also studied by Murray et.al. [13]. A typical nature of the low resolution Raman spectra as observed by Greytak and Yan [11] is depicted in Fig. 5.1, while the high resolution spectrum [12] is shown in Fig.

5.2.

Ohbayashi and Ikushima [14] measured the fine structure of the Raman bands of He-II at svp and observed cusps (cf Fig. 5.3) at $2\Delta_0$, $2\Delta_1$, and $2\Delta_2$ with their energy equal to $17.1 \pm 0.5K$, $27.5 \pm 0.5K$ and $34.8 \pm 0.5K$, respectively. They also observed additional structure whose origin could not be identified. An extensive study of the Raman spectra at 1.37K under svp for three different values of instrumental FWHM (= 1.1k, 1.9K, and 3.7K) has been reported by Ohbayashi and Udagawa [4]. Beside the two strong peaks as observed by Greytak and Yan [11], they also observed an additional structure similar to that reported by Ohbayashi and Ikushima [14]. They also extended their measurements to an energy shift of about 450K with a resolution good enough to observe some structure.

5.3 THEORETICAL MODELS

5.3.1: Models with Non-interacting Excitations

Light interacts with liquid helium through two different interactions: (i) dipole induced dipole (DOD) interaction, and (ii) electron overlap (EO) interaction. The former is concluded to be responsible for d-wave scattering, while the latter leads to s-wave scattering.

Halley [1] was the first to report a systematic theoretical study of RS from liquid ^4He using electronic excitations of a helium atom as intermediate states. His calculations of the amplitude of second order two-roton RS revealed it to have experimentally observable magnitude. Using the experimentally known roton spectrum and the pair correlation function, Halley also calculated the RS cross section as a function of roton energy transfer. He argued that the coupling between an elementary excitation of liquid helium and the electromagnetic field is expected to be very weak, consequently as a first order process, only Brillouin scattering can be observed. The first order Raman process also encounters a problem from momentum conservation. However, this problem does not appear for the observation of second order RS in which two excitations of equal and opposite momenta are created simultaneously. The peak scattering may be expected to occur where the density of states of two excitations is largest; this means that the two excitations involved in the process should correspond to the two closeby points on the flat portion of the $E(q)$ vs. q curve (cf. Fig. 3.1, Curve-A). These peaks in the density of states occur at the same energy in all directions in q space because the liquid is isotropic and one expects peaks at ≈ 17 , ≈ 27 K, or ≈ 37 K due to 2-roton, 2-maxon or 2-plateau modes, respectively. Halley's calculation predicts

Raman peaks due to both 2-maxon and 2-roton modes of nearly equal intensity. However, in the experimental work done by Greytak and Yan [11], no evidence of the 2-maxon peak was reported, they ignored a shoulder around 2-maxon energy.

Stephen [15] developed a semi-phenomenological theory of RS from ^4He liquid using: (i) Lorentz-Lorentz theory of propagation of light in a medium where each atom is assigned with nonzero electric polarizability and (ii) a hydrodynamic approximation for density correlations. He estimated the intensity of light scattering from the 2-roton excitation process to be $\approx 10^{-4}$ times the intensity of Brillouin scattering and this has been found to agree with experimental results. He further concluded that since the intensity of scattered light does not diverge at $2\Delta_0$, (because of the finite lifetime of the rotons) a bound state of the two roton mode of excitations is always expected under such situations and the interaction is attractive. However as pointed out by him, a bound state of two maxons is expected for repulsive interaction as, the effective mass of a maxon is negative. He used these points to show that the calculated Raman intensity of 2-roton peak agrees well with the experimental values [12]. It may be noted that these calculations are greatly simplified by neglecting the interaction of a roton with other excitations.

Nakajima [16] developed an elementary quantum theory of light scattering from liquid helium and presented a generalised formalism of second quantization in which the liquid is assumed to contain ^4He atoms in electronically excited state; the dipolar coupling between excited and normal atoms is included as a perturbation that serves as the source of scattering of photons. Although, the cross sections of Brillouin and RS obtained from this theory agree with the results of Stephen [15], the presence of electronically excited atoms assumed in the liquid at $T \leq 4.2\text{K}$ is a serious weakness of his theory.

Fetter [17] formulated a theory and considered that light scattering in ^4He arises through density fluctuation. By including s-wave scattering process he found a value of 0.69 for polarization ratio differing slightly from the experimental value = 0.74. The calculation of the intensity ratio of RS and BS gave a value $\approx 5 \times 10^{-4}$ which agrees well with experimental value (3.4×10^{-4}) measured by Woerner and Greytak [12].

5.3.2: Models with Interacting Excitations

Theoretical basis for the absence of 2-maxon peak was sought independently by Iwamoto [18] and Ruvalds and Zawadowski [19]. In his approach, Iwamoto considered a final state interaction between

a pair of elementary excitations and pointed out that the RS changes drastically when the excitations produced in the process have small group velocities and showed that there should not be any peaks at these points in spite of the infinite density of states. This observation was interpreted [18] as a destructive interference between the excitations with positive and negative group velocities. He also investigated the possible existence of resonance between two maxons which depends on their interaction around the extremum.

Ruvalds and Zawadowski [19] used Green function technique to investigate interaction between excitations in He-II, and explained the observation of a resonance of two rotons. Interaction of this resonance with single particle spectrum has been shown to produce hybridization and splitting of one particle spectrum into two distinct branches.

A theoretical model by Zawadowski et.al [20] reveals that the pair density of states is drastically altered if the excitations interact. While the attraction increases the density of states of roton pairs, it affects adversely the density of states of maxon pairs, and corresponding band is not observed. However, the ZRS model has been questioned in a recent investigation of Raman

spectra by Udagawa coworkers [5,6]. They have argued that this picture does not account for the structure observed in the Raman spectrum. The ZRS model also violate the excluded volume condition [21]. In addition Nakajima [16] has suggested that direct interaction may be important in the Raman scattering process. Despite a good agreement between theoretical and experimental results, the reliability of the theoretical models are questionable for ignoring certain basic facts about the system recently revealed by Jain's theory.

5.4 RESULTS AND DISCUSSION

It has been observed by Greytak and Yan [11] that the intensity ratio, $R = I(\text{Raman})/I(\text{Brillouin})$, is three orders of magnitude weaker than that of Brillouin scattering from phonons and this agrees with theoretical predictions. R is also found to change linearly with the change in instrumental width and to depend strongly on temperature particularly in the low temperature range of 1.2 to 1.5K.

RS from ^4He liquid is found to be highly depolarised. Stephen explained this observation by using DID model of light-helium coupling [15] leading to d-wave scattering. However, Iwamoto [18] pointed out that s-wave scattering should also be

possible and in this context Nakajima [16] argued that interaction due to direct overlap of wavefunctions of near neighbour atoms should also be important in two roton RS since this causes both s and d wave scattering. Fetter [17] calculated the numerical value of depolarisation ratio (β) by including for s-wave scattering at two roton peak. He obtained $\beta = 0.69$ which falls lower to the experimental value of $\beta = 0.74$. It may be noted that for pure d-wave scattering β is 0.75. Obviously the results of Woerner and Greytak [12] appear to be consistent with d-wave scattering. Kleban and Halley [22] using semi-empirical method and uv-absorption data found that s-wave scattering amplitude should be significant. They further predicted that s-wave contribution should increase with increase in energy shift. Incorporating EVC in their microscopic calculation, Campwell et.al.[23] have shown that integrated intensity ratio of s and d wave scattering has a range 0.08-1.88. Kleban and Halley [22] considering polarization effect found this range to be 0.11-1.45. The experimental value of the ratio = 0.16 ± 0.03 clearly falling in the predicted range, reveals that s-wave contribution are relatively small. The experimental fact that the ratio of s-wave scattering intensity to that of d-wave scattering increases with increasing energy of the Raman shift agrees with theoretical results.

The observation by Greytak and Yan [11] that the 2-roton peak occurs at an energy shift less than $2\Delta_0$ at the same temperature, was interpreted by them as a direct evidence for the existence of a 2-roton bound state. A comparison of the spectra with theoretical calculations gives a binding energy ($\Delta\varepsilon_r$) of 0.37 ± 0.10 K. Using the theory of interacting excitations, Murrey et.al. [13] analysed the experimentally observed 2-roton line shape and concluded that roton-roton interaction energy $\Delta\varepsilon_r = 0.22 \pm 0.07$ K is necessary to explain the observed spectrum. A similar study by Ogita et.al. [7] also reveals $\Delta\varepsilon_r \approx 0.2$ K. High resolution study by Ohbayashi and Ikushima [14], revealing $\Delta\varepsilon_r = 0.5 \pm 0.3$ K, also corroborates the existence of interaction between two elementary excitations of equal and opposite momenta as their general property.

Although, several groups believe in the existence of roton-roton interaction, however, certain groups do not agree on this point [21,22,24]. In this context, we note that Landau-Khalatnikov theory successfully explains the temperature dependence of the roton contribution to viscosity by considering repulsive interaction between two rotons and this does not fall in line with attractive interaction envisaged [7,11,13,14] to account for the observed Raman spectra of He-II. Different explanations

are offered to understand this apparent contradiction. For example: (i) since the experimental values for viscosity are available for limited temperature range, the temperature dependence of viscosity can not be considered reliable, and (ii) formulating a theory of the intensity of RS from liquid ⁴He using dynamical correlation function, Kleban and coworkers [21,22,24] have shown that none of the existing theoretical interpretation of the Raman experiment is reliable because these are not consistent with the "excluded volume condition (EVC)", -a direct consequence of the simple fact that two atoms cannot overlap. Kleban [21] also argues that an experimentally detectable shift of the two-roton peak should be possible due to other reasons. His calculation reveal that possible change in the parameters in his theoretical formulation also gives a shift in the frequency of 2-roton mode to a value as good as 0.24K which is as large as observed experimentally. Thus the deviation of the observed frequency from $2\Delta_0$ does not conclusively suggests the presence of attractive interaction between two rotons.

Noting that the linewidth/lifetime of 2-roton mode originates from collisions with thermally excited rotons, the roton-roton collision time estimated from the experimentally observed temperature variation of the Raman linewidth has been found to

agree with its value estimated from the roton contribution to the normal fluid viscosity. Further since the temperature dependence of the linewidth is determined mainly by the roton number density $n_r(T) = n_r(0) \cdot \exp[-\Delta_0/kT]$, one can estimate the collision time and find information about the roton-roton interaction. For this purpose Landau and Khalatnikov [25] assumed a repulsive potential (represented by the pseudopotential $V_0 \phi(r)$) between two rotons. Using the experimental values of linewidth, this however gives a value of $V_0 = 1.73 \cdot 10^{-38}$ erg cm³ which is found to be an order of magnitude higher than that estimated from the binding energy. Ohbayashi et.al. [6] used one component model with lorentzian temperature-broadening both above and below T_λ and determined Δ_0 and roton lifetime. While Δ_0 was found to exhibit weak temperature dependence as observed experimentally, the roton lifetime was found to deviate from Landau-Khalatnikov theory above 1.80 K.

5.5 OUR ANALYSIS OF THE HIGH RESOLUTION RS SPECTRUM

It has been noted that different pseudopotentials are needed to account for different experimental observations. While the observed bound state as suggested to exist from the observed RS spectrum, requires a weakly attractive pseudopotential, the collision time processes responsible for viscous behaviour of the

liquid requires a repulsive pseudopotential. In this connection we present the following explanation [26]. The quasiparticle rotons could be assumed to behave like real atoms with interparticle potential having two terms: (i) short range repulsive potential and (ii) long range attractive potential. The effective range of repulsion may be as small as the average distance (d) between two ^4He atoms in the liquid, while that of attraction (if exists) could be as large as some multiple of d . This follows from the fact that wavelength corresponding to q value of roton excitation is as small as d and the particles cannot ride over each other even in their excited states where relative motion of neighbouring atoms play the crucial role. It is natural that the attraction is weak and the depth of the potential is shallow. Obviously, in the viscous behaviour of the liquid, the short range repulsive potential is expected to dominate the process. On the other hand, the two rotons created in the process of Raman scattering need not be located within the sphere of repulsive interaction, they are more likely to have separation where they have weak attractive interaction or no interaction at all. An estimate of the of the range of attraction reveals its value to be around 13\AA [2], while the wavelength of the light used to excite Raman scattering ($\approx 5000\text{\AA}$) is much larger than this value. Obviously, though the excitation of two

rotons having separation lower than $13A^{\circ}$ is possible, the probability of exciting two rotons having separation larger than the range of their attraction should be reasonably high. Consequently, we may expect 2-roton peak at an energy which is not perturbed by the attraction between two rotons. Combining this account with the expectation of a peak having two split components concluded for two attractively interacting rotons by Iwamoto [18], we expect a total of three peaks (cf. Fig 5.3) as observed experimentally by Ohbayashi and Ikushima [14]. This agreement not only corroborates the accuracy of our suggestion but also provides an explanation for the unexplained observation of P_3 peak (cf. Fig. 5.3). Accordingly, P_3 arises due to two non-interacting rotons. It may be mentioned that Ohbayashi and coworkers [4,5] have attempted to associate their observation of additional structure in their high resolution spectra to $k=0$ condensate in He-II. The explanation does not agree with the fact that $k = 0$ condensate does not exist in He-II, as per the theory by Jain and its existence has not been proved experimentally beyond doubt.

Numerical calculations of the Raman spectra of He-II by Hasting and Halley [27] reveal that a broad peak should appear at an energy shift corresponding to the 4-roton energy, regardless of the differences in the models. In their calculations, they

assumed three different situations of: (i) no interaction, (ii) a localized interaction, and (iii) a constant interaction between elementary excitations. While these calculations are considered to be unreliable for the violation of EVC [21], the inference that Raman peaks at even multiple of Δ_0 should appear in the spectrum has been considered important by Ohbayashi and Udagawa [4] because the so called $2\Delta_2$ peak observed in the spectra can also be attributed to $4\Delta_0$, and a weak and broad peak for $6\Delta_0$ has been seen at $\approx 52\text{K}$. However, we find that NIS measurements under pressure reveal that the roton energy decreases with an increase of applied pressure and the 4-roton peak is expected to appear at $\approx 29\text{K}$ under a pressure of 20 atmosphere. In variance with this expectation, the observed peak at $\approx 35\text{K}$ does not shift with increasing pressure. This result suggests that we cannot simply associate the observed peak at $\approx 35\text{K}$ with 4-roton mode. Consequently, the existence of this should be carefully examined.

5.6 CONCLUDING REMARKS

It may be noted that extensive experimental study of RS from liquid ^4He has revealed almost all possible aspects it is expected to provide. However, the accuracy of theoretical formulation and their results is still uncertain for several reasons as for example:

(i) The basic nature of He-II for its atomic arrangement was not correctly understood and the theoretical formulations considered it as a system of atoms which move randomly like those in normal fluids.

(ii) The atomic dynamics defining various modes of excitations was not precisely understood; obviously, the accuracy of calculations of the amplitude of RS and hence the Raman intensity remains uncertain.

(iii) As pointed out by Kleban [21] the calculations violate the basic consequence of excluded volume condition and thus conclude that the calculations are unreliable. Further several additional structures observed in high resolution spectra are not explained by the theoretical models proposed in the literature.

From our analysis, we conclude the following (a) a shoulder due to 2-roton which was overlooked by others is actually clearly visible. (b) the unexplained peak at P_3 [14] was explained by us as due to two non-interacting rotons and (c) the existence of the 4-roton peak at around 35K [4] was ruled out.

We therefore, hope that a better understanding of Raman

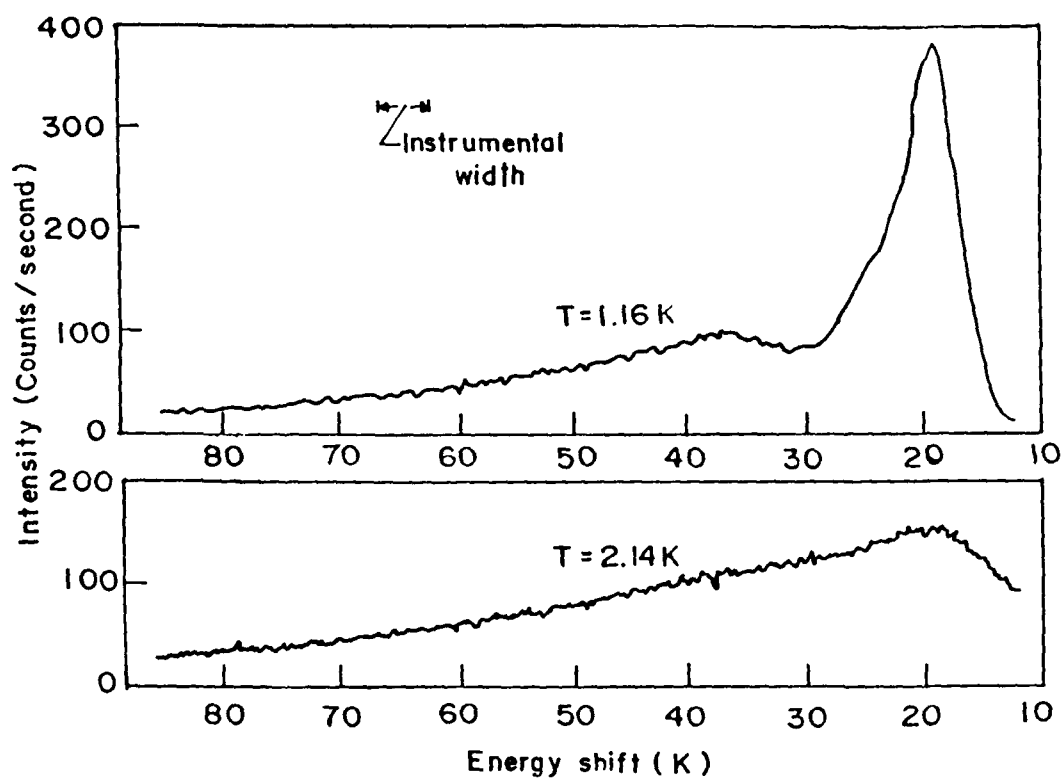
scattering results can be achieved if the model proposed by Jain [28] is used in the theoretical formulation of the Raman scattering from He-II. It may therefore be suggested that attempts should be made to formulate a theory of Raman scattering from He-II which includes the new information on the space and momentum configuration of He atoms in He-II and modified EVC.

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. 5.1: Low resolution Raman Spectrum as observed by Greytak and Yan [11]

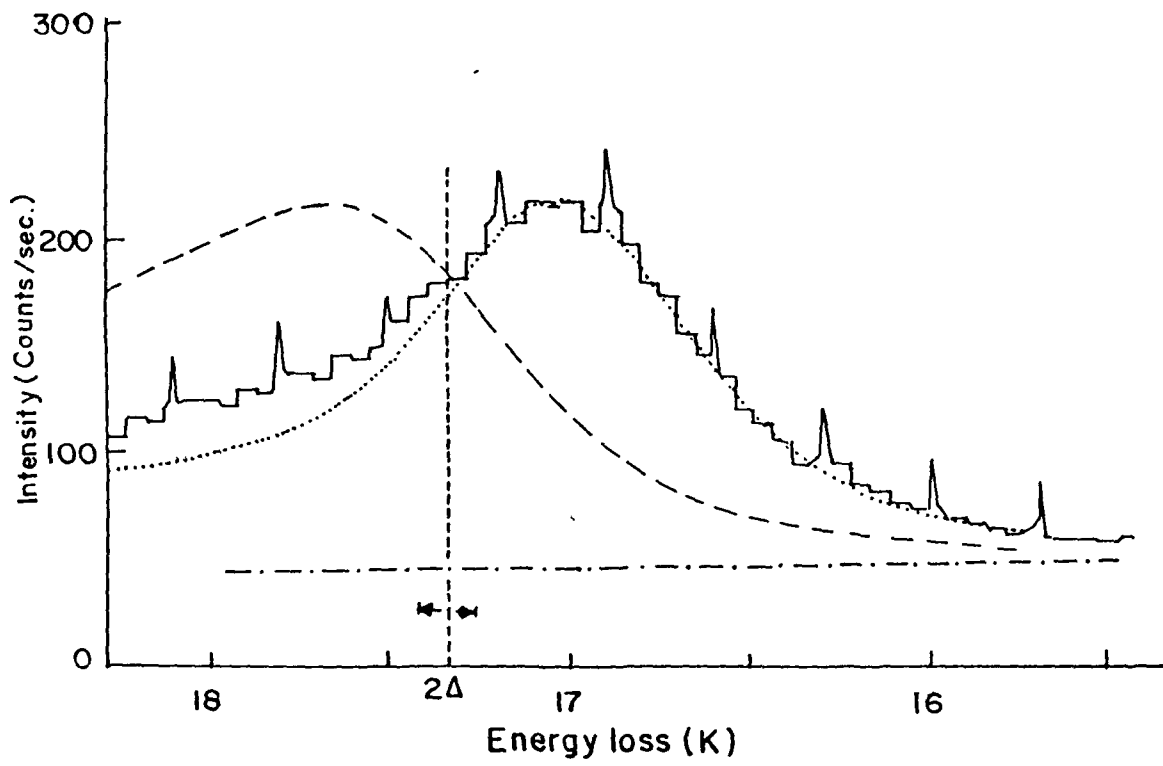


Fig. 5.2: High resolution Spectrum [12].

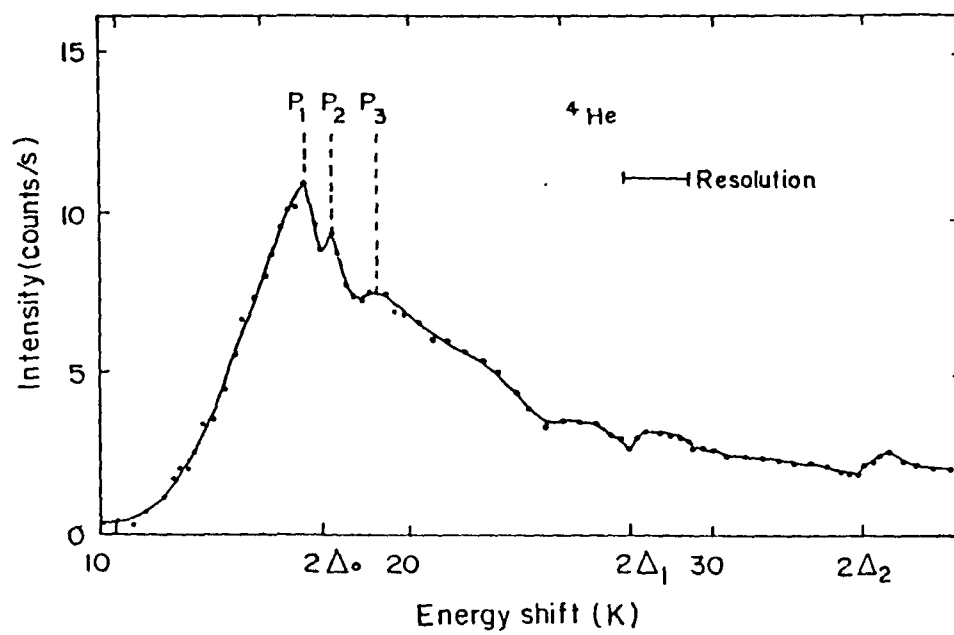


Fig. 5.3: Fine structure spectrum as observed by Ohbayashi and Ikushima with cusps at $2\Delta_0$, $2\Delta_1$ and $2\Delta_2$ [14]

CHAPTER: VI

CONCLUDING REMARKS

In nature there exists certain systems whose macroscopic behaviour changes drastically as one goes to low temperature and a superfluid belongs to one of them. A Superfluid reflects the operation of quantum nature at macroscopic scale and it was pointed out by London and London [1] that the mechanics which superfluid follows must be quite different from that of the classical fluid.

London [1] observed that superfluid belongs to a system in which a macroscopic fraction of the particles are locked into the ground state and it is this observation which gave rise to the so called two fluid theory. The de Broglie wavelength of particle in the superfluid phase was considered to be infinite and in a confined system it could be as large as the size of the container.

The most successful macroscopic theory was presented by Landau [2]. The Landau's Two fluid theory supplemented by Onsager quantization [3] forms the basis of the macroscopic description of He-II. It was further modified by including dissipation effects which comes into play when the liquid flows. However it must be mentioned that certain conclusion drawn from the macroscopic quantum theory are inconsistant with the theory proposed by Landau and thus a single theory which unifies the macroscopic quantum

ideas with that of the two fluid is a must. In this context one finds that a microscopic theory developed by Jain fills this gap and vindicates two fluid theory of Landau and explains all important properties of ^4He .

While analysing the flow of ^4He Allen et.al [4] and Kapitza [5] found that at low temperature, the liquid helium could flow through narrow capillaries without friction. Other measurements based on oscillatory disc and rotational viscometer, however, shows finite value of viscosity and this gives rise to a paradox. The paradox was removed by considering two fluid motion, where the cause of viscosity is the normal component of the fluid. In a narrow capillary, the normal component is clamped and thus do not flow and hence there is no question of viscosity. The presence of viscosity in other methods is due to the flow of the normal component. While the same conclusion are imminent from Jain's microscopic theory [cf chapter II] as it provides the microscopic basis to the two fluid theory, however, Jain's theory reveals more than this. We note that in SMW configuration, particles are trapped in antinodal regions of SMW waveform and they do not move across the particles, partially when they are moving in narrow channels. As such the particles in these channels lose their relative motion, the main cause of viscosity. In rotatory

viscometer the particles form concentric circles on which they move with different relative velocity and naturally we observe the game of viscous forces.

Experimental results obtained by Reppy [6] indicates that the superfluid component do take part in rotation. But, as one knows there should not be any rotation for a conserved system, this gives rise to a paradox. This paradox was removed by considering the presence of vortex singularities which rotates keeping the equilibrium state stationary. The theory as proposed by Jain also supports the existence of quantised vortices which so far was understood in terms of the phenomenological argument by Feynman. However it must be pointed out that Feynman's explanation is equally valid for normal fluid. But the existence of any quantum vortices was not found in the normal phase. The Jain's microscopic theory, however, distinguishes the two phases as ordered and disordered particles in the phase space and further shows that quantum vortices can be sustained only in the ordered phase i.e the superfluid.

It was pointed out by Putterman [7] that liquid Helium might perhaps provide a strongest check of the Schrodinger wave equation. However the fact is that no unified microscopic theory

could emerge to account for the unique properties of He-II. Putterman speculated that the present theory of nature (the wave mechanics) may not have the basic principles necessary for understanding the behaviour of He-II. Although Jain's theory has been developed in the frame work of the wave mechanics yet Putterman was right in his contention as the intricacies of wave mechanical uncertainties were not rightly understood; as a result of which all efforts fail to achieve the goal of developing the desired theory of He-II.

A study of the dynamical behaviour of He-II reported in this thesis uses the basic fact revealed from the microscopic theory of interacting bosons (such as ^4He atoms) recently developed by Jain (cf. chapter - II). Accordingly, He-II in its ground state is a close packed system of particles wavepackets which could be identified to have a symmetry of hcp/fcc etc. It naturally reveals that with a change in energy and momentum of the particles under the influence of thermal excitation, the size of the wavepackets decreases and this causes an increase in the inter-particle force constant (C) and decrease in the inter-particle separation (d). This aspect has been used to analyse the unexplained anomalous nature of the observed excitation spectrum of He-II.

To study the excitation spectrum in the lower q region, we approximated the system as a monoatomic linear chain of atoms. As the system is isotropic, the longitudinal modes are identical. The shear force is negligibly small, the transverse modes are thus omitted. However, as the value of C and d are no longer fixed as in the case of a rigid crystalline system, we find that they are the ascending and descending functions of q respectively. We studied the q dependence of C and d and used these results to calculate V_p (phase velocity), V_g (group velocity) and E_{ph} (phonon energy). The values of these entities thus obtained agree very well with the experimental results, revealing the origin of the anomalous nature of V_p and V_g .

The variation of the roton position (q_0) and energy (Δ) with density forms an interesting aspect of study which helps in understanding several interesting properties of He-II. We investigated this aspect and our results are found to match very well with the experimental values.

The region beyond $q > q_r$ (refer. Fig. 3.1) can be identified with that of the free particle motion, as the wavelength associated with the particles becomes shorter than the size of inter-particle separation. As q increases further, the spectrum

is observed to get modified. We have explained this observation as due to mixing of the free particle nature with that of the multiphonon mode and determined that an interaction of 4.5K explains the observed spectrum to a very good approximation.

A connection between the structure factor and the spectra of elementary excitations was determined by Feynman. However, the calculated spectrum was found to have values which are about twice of those observed experimentally. This discrepancy is logically removed from the fact revealed from the Jain's microscopic theory which concludes a smw pair of mass $2m$ to be the basic unit of the system. We find that results obtained by using $2m$ instead of m in the Feynman's formula match very well with values in the experimentally observed curve.

We also calculated the value of the first, second and the fourth sound in He-II. In order to obtain the expression for the first sound, we used the relation as predicted from the microscopic picture, but with certain modifications to account for the change in the structure and symmetry due to the applied pressure. Calculations were done as a function of pressure and results, thus obtained agree with the experimental results.

To calculate the second sound we applied the relation between c_2 and ρ_s as obtained by Landau. The value of ρ_s and ρ_n (as required in the expression) were obtained after normalizing the superfluid density with energy-gap, a fact established in the microscopic theory. These values were then applied in the relation for the second sound. The results thus obtained agree to a great extent with those reported in literature.

The density of superfluid (ρ_s) was also calculated from the velocity of third sound. The nature of ρ_s obtained establishes the fact that E_g (the energy gap) vanishes at the boundary.

Finally to obtain the velocity of the fourth sound we used our values of first and second sound velocity and the observed curve is found to match very well with the experimental curve.

The dynamical aspects of He-II as observed by Raman Spectra has been analysed successfully along with a comprehensive review. The presence of certain fine bands as observed under high resolution has been satisfactorily explained.

We thus see that the detailed analysis of several interesting properties of He-II, which could not be explained so far for the

want of a comprehensive microscopic theory, have been successfully explained by the unified microscopic theory as proposed by Jain. Many other interesting properties of He-II like surface tension, infinitely high thermal conductivity, quantum vortices and related properties, can also be understood not only at the qualitative level but also at the quantitative scale by using his microscopic model and this will form our future plan of research. This picture would further provide an insight into the system of spin-polarised hydrogen and also provide better knowledge about the superfluidity of liquid ^3He , whose properties are much more complex and diverse than those of ^4He . This picture may also open doors for better understanding of the physics of creating superfluid exciton liquid in semiconductors, superfluidity in a vacancy gas in quantum crystals like solid helium or solid molecular hydrogen, superfluid state of ^3He dissolved in ^4He as an impurity, superfluids of liquid molecular hydrogen under certain condition like negative pressure and supercooling, superconductors, nucleus and neutron star.

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