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Theory of excitations in superfluid $^4$He: an introduction

The major goal of the present book is to outline the field-theoretic analysis of the dynamical behaviour of a Bose-condensed fluid that has developed since the late 1950's. While we often use the weakly interacting dilute Bose gas (WDBG) for illustrative purposes, the emphasis is on the dynamical properties of a specific Bose-condensed liquid, superfluid $^4$He. We attempt to develop a coherent picture of the excitations in liquid $^4$He which is consistent with, and rooted in, an underlying Bose broken symmetry. Recent high-resolution neutron-scattering studies in conjunction with new theoretical studies have led to considerable progress and it seems appropriate to summarize the current situation. The only other systematic account of superfluid $^4$He as a Bose-condensed liquid is the classic monograph by Nozières and Pines (1964, 1990).

The phenomenon of Bose condensation plays a central role in many different areas of modern condensed matter physics (Anderson, 1984). Historically it was first studied in an attempt to understand the unusual properties of superfluid $^4$He (London, 1938a). In a generalized sense, however, it also underlies much of the physics involved in superconductivity in metals and the superfluidity of liquid $^3$He, in which Cooper pairs play the role of the Bosons (see, for example, Leggett, 1975 and Nozières, 1983). In recent years, there has been increased research on the possibility of creating a Bose-condensed gas, involving such exotic composite Bosons as excitons in optically excited semiconductors, spin-polarized atomic Hydrogen, and positronium atoms. This research, in turn, has re-stimulated theoretical interest in Bose condensation in general and its implications in both liquids and gases.

Although $^4$He was first liquefied by Kammerlingh Onnes in 1908, it was not until 1928 that Wolfke and Keesom found it could exist in two phases, now called Helium-I and Helium-II, separated by the transition
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Fig. 1.1. The P-T diagram for the condensed phases of $^4$He contrasted to that for a normal liquid.

temperature $T_s = 2.17$ K at SVP. Kapitza (1938) and, independently, Allen and Misener (1938), found that the fluid flowed without any apparent viscosity below $T_s$. At higher temperatures ($T > T_s$), the liquid exists as a “normal” liquid and is called liquid Helium-I. Below $T_s$, liquid $^4$He is a “superfluid” (a term introduced by Kapitza for a fluid having, in a certain sense, zero viscosity) and is called Helium-II. Most of our discussion will deal with this low-temperature superfluid phase, but we will also be interested in how it differs from Helium-I (above $T_s$). The phase diagram is shown in Fig. 1.1.

The study of superfluid $^4$He has played a central role in developing our understanding of many-body systems. The modern idea of quasiparticles started with Landau’s original theory of superfluid $^4$He (1941). Bogoliubov’s (1947) derivation of the phonon spectrum in a weakly interacting dilute Bose gas was one of the first treatments of a broken symmetry. In this chapter, we give a brief review of theories about the excitations of superfluid $^4$He and how they developed since the pioneering work of London, Tisza, Landau, Bogoliubov and Feynman. In this mini-history, we also introduce the kind of questions with which the rest of this book will be concerned. We assume the reader is already familiar with an elementary account of the properties of superfluid $^4$He, such as the first three chapters of Nozières and Pines (1964, 1990). In Section 1.1, we sketch the well known Landau–Feynman quasiparticle picture (which makes no reference to an underlying Bose condensate). In Section 1.2,
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we review the development of the theoretical approach in which the condensate plays a crucial role. It is with this latter approach that this book is concerned.

Many experimental probes have given valuable information about the excitations in superfluid $^4$He, including Brillouin and Raman light scattering, sound propagation, as well as thermodynamic and transport studies. However, the most powerful technique has been inelastic neutron scattering. Through the dynamic structure factor $S(Q,\omega)$, this is a direct probe of the density fluctuations which turn out to be the elementary excitations of superfluid $^4$He (but not, as we shall see, of normal liquid $^4$He). Moreover, recent high-resolution neutron-scattering data over a wide range of temperatures and pressures have stimulated the theoretical developments which are a major theme of this book. For these reasons, we shall discuss neutron-scattering data at some length. As background, we summarize in Chapter 2 some general properties of the dynamic structure factor which hold for any system and also the main features that $S(Q,\omega)$ exhibits in superfluid $^4$He. References to neutron-scattering results in the overviews given in Sections 1.1 and 1.2 are more fully explained in Chapter 2. For a general account of experimental studies on excitations in superfluid $^4$He, the classic review article by Woods and Cowley (1973) is highly recommended.

In Section 1.3, we conclude with an extended outline of the contents of the succeeding chapters of this book.

1.1 Landau–Feynman picture

The superfluid characteristics of Helium-II are well described by the two-fluid model, first suggested by Tisza (1938) and later brought to fruition by Landau (1941). In this model (for authoritative accounts, see Landau and Lifshitz, 1959; Khalatnikov, 1965), the liquid consists of two interpenetrating fluids, a normal fluid and a superfluid, each having its own density and velocity fields. The normal fluid has a finite viscosity, contains all the entropy of the liquid, and has a mass density $\rho_N$ and velocity $v_N$. The superfluid component has no entropy and it has a mass density $\rho_S$ and a velocity $v_S$. If $v_S$ is less than some appropriate critical velocity, the superfluid component flows with zero viscosity. The local mass density and the momentum current density are given by the equations

$$\begin{align*}
\rho(r) &= \rho_N(r) + \rho_S(r), \\
\mathbf{J}(r) &= \rho_N(r)v_N(r) + \rho_S(r)v_S(r).
\end{align*}$$

(1.1)
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In He-II, the normal fluid fraction $\rho_N/\rho$ is a strong function of temperature. As the temperature decreases, the normal fluid fraction goes to zero. Above $T_c$, the normal fluid fraction is unity, corresponding to the fact that there is no superfluid component. There are many ways of measuring $\rho_S$ and $\rho_N$, but the most precise experimental results are from measurements of $\rho_N$ from the moment of inertia of a rotating disk (Wilks, 1967).

The two-fluid model, consisting of (1.1), the continuity equation, and a set of three other equations describing the flow produced by gradients in the temperature, pressure, and chemical potential, has been extremely successful in describing the macroscopic transport properties and the low-frequency, low-wavelength hydrodynamic modes in Helium-II (Khalatnikov, 1965). One of the great successes of the field-theoretic analysis of Bose-condensed fluids (see Chapter 6) is to show how this two-fluid description can be a natural consequence of a Bose order parameter (Bose condensation).

London (1938a,b) proposed that superfluidity in liquid $^4$He is a manifestation of Bose–Einstein condensation. Tisza (1938) also conjectured that the superfluid component in his phenomenological two-fluid model could be interpreted as the fraction of the Helium atoms that are Bose-condensed. As we discuss in more detail in Chapters 4 and 6, the condensate fraction and the superfluid fraction are not the same in a Bose-condensed liquid like superfluid $^4$He. At zero temperature, the superfluid fraction is 100% (since no quasiparticles are thermally excited) while the condensate fraction is only about 9%. In his classic papers of 1941 and 1949, Landau strongly argued against any connection between a Bose condensate and the two-fluid model. The modern view vindicates both Landau and London in that the microscopic basis of Landau’s quasiparticle picture and the two-fluid description lies in the existence of a Bose condensate.

The Landau (1941, 1947) theory of superfluidity is based on the low-lying excited states of a Bose liquid. He showed that the low-temperature thermodynamic and transport properties of superfluid $^4$He could be understood in terms of a weakly interacting gas of Bose “quasiparticles” (phonons and rotons). This description is in many ways analogous to the phonon picture of an anharmonic crystal (see Chapter 11). This was developed at some length by Peierls, Frenkel and others in the early 1930’s. In superfluid $^4$He, Landau had no well defined scheme to calculate the dispersion relation of the quasiparticles; i.e., how to relate it to the microscopic forces between the $^4$He atoms. Although certain qualitative features could be argued to be consequences of the Bose
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statistics of the $^4$He atoms, the dispersion relation of the quasiparticles in superfluid $^4$He was viewed by Landau (1947) as something to be determined from experiment. We recall his strong resistance (Landau, 1941, 1949) to trying to use a WIDBG as a model for superfluid $^4$He, as London (1938a,b) and Tisza (1936) tried to do. A quasiparticle spectrum which was acoustic at low $Q$ but has a roton minimum at large $Q$ has precisely the features needed to explain the temperature dependence of two-fluid thermodynamic functions as well as the velocities of first and second sound. In the two-fluid picture, the normal fluid density describes the thermally excited quasiparticles, while the superfluid density can be thought of (in a rough sort of way) as the probability that the liquid is in its ground state.

At low temperatures ($T \sim 1$ K), the dominant feature of the dynamic structure factor $S(Q, \omega)$ in the range $0.1 \text{ Å}^{-1} < Q < 2.4 \text{ Å}^{-1}$ is an extraordinarily sharp resonance. This is illustrated by the representative data in Fig. 1.2 as well as in many other figures in this book. (It is to be emphasized that plots of $S(Q, \omega)$ data almost always still contain instrumental resolution broadening, with a width typically of order 1–2 K.) As first pointed out by Cohen and Feynman (1957), the peaks in $S(Q, \omega)$ correspond to the creation of the elementary excitations which Landau (1941, 1947) originally postulated to describe the thermodynamic and transport properties of superfluid $^4$He. The roton was first observed using neutron scattering by Palevsky et al. (1957). The complete quasiparticle dispersion relation $\omega_Q$ (see Fig. 1.3) was first determined by Yarnell, Arnold, Bendt and Kerr (1959) and Henshaw and Woods (1961) at $T = 1.1$ K. For $Q$ values below about 0.6 Å$^{-1}$, the dispersion relation is phonon-like ($\omega_Q = cQ$), with a slope slightly larger than the thermodynamic speed of sound. It bends slightly upward (anomalous dispersion) before bending over to a maximum energy (referred to as the “maxon”) of about 14 K at $Q_M = 1.13$ Å$^{-1}$. The minimum at $Q_R = 1.93$ Å$^{-1}$ occurs at an energy $\Delta = 8.62$ K at SVP. The dispersion relation near the minimum is called the “roton” region. For $Q$ within about 0.25 Å$^{-1}$ of $Q_R$, $\omega_Q$ is found to be very well described by the simple Landau expression (Woods, Hilton, Scherrn and Stirling, 1977)

$$\omega_Q = \Delta + \hbar(Q - Q_R)^2/2\mu_R$$

(1.2)

where the roton “mass” is $\mu_R = 0.13m$ ($m$ is the bare mass of a $^4$He atom).

An important early study by Bendt, Cowan and Yarnell (1959) showed that various thermodynamic functions of superfluid $^4$He up to about
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Fig. 1.2. A plot of the neutron-scattering intensity vs. the energy at a momentum transfer $Q = 1 \text{ Å}^{-1}$, as a function of the temperature [Source: Stirling, 1991; Andersen, Stirling et al., 1991].

1.8 K could be calculated (with an accuracy of a few per cent) by treating it as a non-interacting gas of Bose quasiparticles with the $\omega_Q$ dispersion relation determined by the peak position in $S(Q, \omega)$ measured at 1.1 K. This work is an empirical proof that, at least up to 1.8 K, the resonances in $S(Q, \omega)$ do indeed give the energies of the elementary excitations of superfluid $^4$He. This is not the case in normal liquid $^4$He or in liquid $^3$He.

In his original paper, Landau (1941) introduced phonons and rotons as two quite distinct kinds of excitations. However, beginning with a later addendum (Landau, 1947), it has been traditional to assume that the quasiparticle spectrum in Fig. 1.3 describes a single excitation branch $\omega_Q$. From this point of view, while different parts of the dispersion curve are described as phonons and rotons, they are not thought to be qualitatively different types of excitations. In spite of this, while the physics behind the phonon part has been viewed as “obvious” (i.e., a compressional sound wave), the physical nature of the roton has been the subject of much discussion over the years (see, for example, Feynman, 1954; Miller, Pines and Nozières, 1962; Chester, 1963, 1969, 1975).
The region around $Q \sim 1 \text{Å}^{-1}$ is often referred to as a “maxon”. This region, however, has such a high energy ($\sim 14$ K) that maxons are never thermally excited and thus they play no direct role in the thermodynamic or transport properties of superfluid $^4$He.

In a rotating vessel of Helium-II, only the gas of excitations rotates with the vessel; thus the angular momentum of the excitations determines the moment of inertia of the system. At temperatures less than about 1 K, when there are few excitations thermally excited, the moment of inertia is greatly reduced from the classical prediction that the entire liquid rotates with the vessel. Landau (1941) was able to express the normal fluid density $\rho_N$ explicitly in terms of the Bose distribution function $N(\omega)$ of the thermally excited phonon-roton excitations,

\[
\rho_N(T) = \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{3} \left[ \frac{\delta N(\omega_p)}{\delta \omega_p} \right]. \tag{1.3}
\]

The normal fluid fraction $\rho_N(T)$ turns out to be a useful quantity since
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It gives an effective measure of the number of quasiparticles thermally excited at a given temperature. At $T = 0$, of course, $\rho_N = 0$ and the entire superfluid component consists of the liquid. Below $T \lesssim 0.6$ K, the low-energy, long-wavelength phonon excitations make the dominant contribution to $\rho_N$ (we note that $\omega \phi \sim 1$ K at $Q \sim 0.1$ Â⁻¹). On the other hand, $\rho_N/\rho$ is very small until the temperature reaches about 1.2 K, and then the thermally excited rotons make the overwhelming contribution. The roton’s relatively high energy ($\Delta \sim 8$ K) is compensated by the high density of states at $Q \sim Q_R$. Finally, at about 1.7 K or so, the quasiparticle damping becomes appreciable and one expects that the simple non-interacting quasiparticle gas picture, and hence (1.3), will increasingly break down as we approach the lambda point $T_\lambda = 2.17$ K (SVP).

Landau (in collaboration with Khalatnikov) also developed the formalism of “quantum hydrodynamics” to calculate the effect of weak quasiparticle interactions (three-phonon and four-phonon processes, phonon–roton scattering, etc.) and to use these results to obtain the temperature dependence of the characteristic transport coefficients associated with the normal fluid (the interacting gas of quasiparticles). At temperatures $T \lesssim 1.7$ K, the Landau–Khalatnikov picture gives a very satisfactory account of the transport properties of superfluid $^4$He, as described in detail in the well known monographs by Khalatnikov (1965) and Wilks (1967).

Landau was the first to make a clear distinction between collective modes (such as first and second sound) and elementary excitations (the phonon–roton quasiparticles). In particular, Landau emphasized that the phonon quasiparticle is conceptually quite different from the first sound hydrodynamic mode, even though the speeds are quite close in magnitude. This distinction between collective modes and quasiparticles is equally important in Fermi liquids like normal liquid $^3$He (see Chapter 1 of Lifshitz and Pitaevskii, 1980) and was later incorporated into the description of the excitations of an anharmonic crystal (see Chapter 11).

The microscopic basis of Landau’s picture was developed by Feynman in the period 1953–1957. Feynman dealt directly with the excited states of a Bose liquid, as opposed to Bogoliubov’s work on the excitations of a Bose gas. Feynman (1953b, 1954) showed that if atoms obeyed Boltzmann statistics, he could construct wavefunctions describing the motion of a single atom with energy $Q^2/2m^*$, where $m^*$ is some effective mass arising from the interactions with other atoms. On the other hand, he found that even at low $Q$, such single-particle states develop...
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an energy gap (relative to the energy of the liquid in its ground state). This gap is a result of the required Bose symmetry of the wavefunction (a pairwise interchange of atoms does not alter the wavefunction) and the fact that in a liquid, motion of an $^4$He atom requires that other nearby atoms move out of the way. Feynman estimated that this single-particle energy gap is of the order of the potential well depth any given $^4$He atom moves in ($\sim 10$ K). In contrast with these high-energy single-particle-like excited states, the excited states corresponding to collective long-wavelength density fluctuations (which involve a large number of atoms moving a small amount coherently) had a sound wave dispersion relation. These brilliant papers by Feynman (1953b, 1954) still deserve careful study. For an assessment of Feynman’s work on liquid $^4$He from a modern perspective, see Pines (1989). For a lucid summary, we refer to the discussion by Wilks (1967).

Feynman (1954) presented a variety of physical arguments to the effect that the excited-state wavefunctions are all described by the expression

$$|\Phi_r\rangle = \sum_{j=1}^{N} f(r_j) |\Phi_0\rangle,$$

(1.4)

where $|\Phi_0\rangle$ is the ground-state many-particle wavefunction and the sum is over the position operators $r_j$ of the $^4$He atoms. Carrying out a $T = 0$ variational calculation with (1.4), it is found that $f(r_j) = \exp(iQ \cdot r_j)$ minimizes the total energy. Since the Fourier transform of the density operator $\hat{\rho}(r)$ is (see Section 2.1)

$$\hat{\rho}^+(Q) = \sum_{j=1}^{N} e^{iQ \cdot r_j},$$

(1.5)

this means that the Feynman ansatz (1.4) corresponds to the creation of a single density fluctuation of wavevector $Q$. The energy of this state (relative to the ground state $|\Phi_0\rangle$) is found to be given by the Feynman–Bijl relation

$$\omega_Q^F = \frac{\epsilon_Q}{S(Q)},$$

(1.6)

where $\epsilon_Q = Q^2/2m$ and $S(Q)$ is the static structure factor (a quantity whose importance had only recently been emphasized by van Hove (1954) at the time of Feynman’s work). Feynman made the following, logically distinct, remarks concerning $|\Phi_r\rangle = \hat{\rho}^+(Q)|\Phi_0\rangle$:

(a) Considering $Q$ as a variational parameter, (1.6) has a local minimum
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at $Q \simeq Q_0 = 2\pi/r_0$ corresponding to the local maximum in $S(Q)$. Here $r_0$ is the mean distance between the $^4$He atoms.

(b) In the limit of low $Q$, (1.6) can be shown to give the correct energy of a state with a single phonon present.

(c) $|\Phi_T\rangle = \hat{\rho}^+(Q)|\Phi_0\rangle$ is an exact eigenstate of the total momentum operator, which commutes with the total Hamiltonian. It follows that (1.6) gives an upper bound to the energy of any excited state with momentum $Q$.

These three arguments led Feynman to suggest that $|\Phi_T\rangle = \hat{\rho}^+(Q)|\Phi_0\rangle$ is a good approximation for an excited state of momentum $Q$ at all values of $Q$. Somewhat surprisingly, the variational ansatz of Feynman describes the low-energy, long-wavelength collective phonon modes and the high-energy, short-wavelength roton modes (which are more single-particle-like). As even Feynman (1954) noted, while the quite different atomic motions involved in phonons and rotons seem to be captured in his wavefunction, it does not appear to shed much light on the microscopic nature of a roton. The question “what is a roton?” has been a recurring one in superfluid $^4$He research (see also Section 12.1).

If the exact excited states are approximated by Feynman’s wavefunctions $|\Phi_T\rangle$, the $T = 0$ dynamic structure factor (see Section 2.1) is trivially given by

$$S(Q, \omega) = S(Q) \delta(\omega - \omega_Q^0).$$

(1.7)

Since we are assuming that the exact eigenstates are density fluctuations, the resulting density fluctuation spectrum (1.7) is a delta function at $\omega_Q^0$. By generalizing the variational form (1.4) to include the possibility of creating an admixture of two density fluctuations (Feynman and Cohen, 1956; Miller, Pines and Nozières, 1962), one is led to improved approximations to the excited states which include “backflow” effects. In sophisticated versions of this kind of calculation (see, for example, Manousakis and Pandharipande, 1984, 1986), the predicted quasiparticle spectrum is in good agreement with the experimental dispersion curve shown in Fig. 1.3. In addition, such studies give rise to the kind of high-energy multiparticle structure exhibited by $S(Q, \omega)$ at low temperatures. This variational approach is referred to as the correlated-basis-function (CBF) method and is reviewed by Woo (1976) and Campbell (1978). We discuss such calculations further in Section 9.1.

Feynman’s penetrating analysis of the low-lying excited states of superfluid $^4$He makes crucial use of Bose statistics in constructing wavefunc-