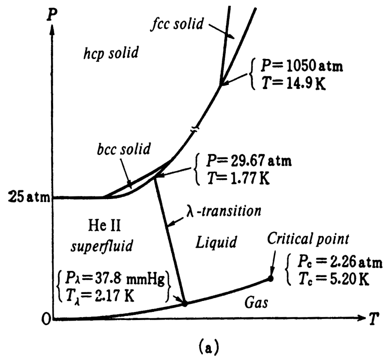

Figure 1: The phase diagram of ^{4} He.

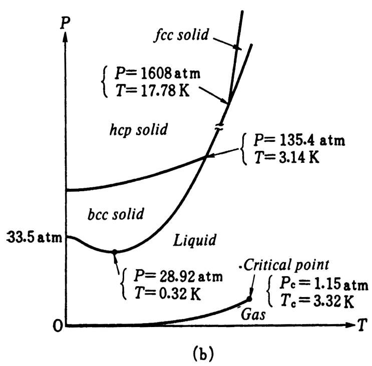

Figure 2: The phase diagram of ^{3} He.

Application of the second quantization method: Phonons

Key Concepts:

Adiabatic continuity, elementary excitations; Broken symmetry; Goldstone nodes; rigidity; wave function.

He3 is one of the simplest fermi systems that can be studied in the laboratory. It has 2 electrons in a closed shell and behaves like a fermion, spin $^1/_2$ particle since its nuclei contain 2 protons and one neutron coupled to spin $^1/_2$.

The other common isotope of the He4 has 2p and 2s with zero net angular momentum, it behaves very differently at low temperature as discussed in a later section (see picture).

The interaction between two He atoms can be modified by a Lenard Jones interaction, describing a hard core repulsive due to the Pauli principle and a week Van der Waals interaction at long distances

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad , \tag{1}$$

whereσ is of the order of the atomic radius 2.5 Å and the scale of the interaction is of the order 10K. The parameter is such that $V(r)$ has no bound states but has a low-lying response (almost bound state) leading to a rapid variation of the phase shifts at low energy. Quantum effects are important where the De Brogile wavelength $\lambda(\frac{1}{2m\lambda^2} \equiv KT)$ is of the order of $\lambda = 7$ Å at 10K.

If we ignore the superfluid phase, which occurs at very low temperature, we find that at low temperature the system is either at fluid or a solid depending on pressure.

The detailed understanding of these two phases is one old and still open problem in the theory of strongly correlated systems.

Two scales are important: σ sets the characteristic "cage size" in which the He3 atom moves, while ε sets the scale of the binding. $\frac{h^2}{2m\sigma^2}$ is a kinetic energy of the particles and the ratio $\frac{h^2}{2m\sigma^2\varepsilon} = \Lambda$ determines the importance of quantum effects.

If $\Lambda \gg 1$ there is no liquid phase;

If $\Lambda \ll 1$ there is a solid at zero temperature at zero pressure. For $\Lambda \sim 1$ the system does not solidify at zero temperature. The Hamiltonian modeling He3 is easily written down using our second quantized formalism:

$$H = H_0 + H_1 \quad , \tag{2}$$

$$H_0 = \sum_{p,\sigma} \varepsilon_p a^\dagger_{p\sigma} a_{p\sigma}. \tag{3}$$

For H4 the spin index is omitted.

$$H_1 = \frac{1}{2V} \sum_{p_1,p_2,p_3,p_4} a^\dagger_{p_1\sigma} a^\dagger_{p_2\sigma} a_{p_3\sigma} a_{p_4\sigma} V(p_4 - p_3) \delta_{p_1+p_2+p_3+p_4}, \tag{4}$$

or in first quantized notation:

$$H_0 = \sum_i \frac{p_i^2}{2m}, \tag{5}$$

$$H_1 = \frac{1}{2} \sum_{i \neq j} V(r_i - r_j). \tag{6}$$

The existence of two phases at T = 0 can be understood from simple dimensional arguments. The kinetic energy term scales at $\frac{p_F}{2m} \sim \frac{n^{2/3}h^2}{2m}$ while the interaction energy scales as $\varepsilon n \sigma^3$. Therefore at low densities H_0 is the dominant interaction and the system is a fluid. At high densities H_1 is dominant. From its first quantized expression, we have to minimize the potential energy without worrying too much about H_0 , and the resulting structure is a FCC crystal.

Both solid and liquid helium three are in a regime where $H_0 \sim H_1$ and serves as a beautiful example of a strongly correlated system, i.e. a system in neither itinerant nor the localized aspects of the physics need to be taken into account.

There are two aspects to this problem, a) the accurate evaluation of the ground state energy per particle of both phases to determine the phase diagram; b) the qualitative understanding of the low energy properties (low lying excitations and long distance behavior of the correlation function in both phases).

(a) is a very hard problem and is to a large degree independent of (b). This is because the short-range correlations, which determine almost the full total energy, are independent of He3 and He4 at low temperature in both the solid and fluid phase have a similar density correlation function at short distances.

The best variational wave function to date has completely wrong distance behaviour.

While these are very important facts seem well established in He3 quantum magnetism, the energy difference between RVB and Neel type of wave functions is also very small.

To answer the questions rose in (b) the ideas of adiabatic continuity and broken symmetries are essential.

Understand the solid phase, imagine that one starts from very high densities and one can neglect H_0 compared to V .

The ground states V is $|R_1 ... R_N\rangle$ where R_i minimize the classical energy $\sum\limits_{i \neq j} V(R_i - R_j)$.

The minimum is a crystal with $R_i \sim \sigma$. If we turn on H_0 the particles will not stay completely localized but if $H_0 \ll V$, the coordinates r_i will not depart two much from R_i . In these circumstances we will show that we can neglect the antisymmetry requirement of the wave function.

We write $r_i = R_i + U_i$,$U_i \ll 1$ and expand to quadratic order.

$$H \simeq \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j} \sum_{\alpha\beta} \frac{1}{2} \frac{\partial^2 V}{\partial r_i^\alpha \partial r_j^\beta} (U_i^\alpha - U_j^\alpha)(U_i^\beta - U_j^\beta) + E_0 + O(U_3), \tag{7}$$

defining:

$$C_{(r_i - r_j)\ \alpha\beta} \equiv \begin{cases} -\frac{\partial^2 V}{\partial r_i^\alpha \partial r_j^\beta}(r_i - r_j),\ i \neq j \\ \sum\limits_j \frac{\partial^2 V}{\partial r_i^\alpha \partial r_j^\beta}(r_i - r_j),\ i = j \end{cases},$$

(7) can be diagalized by a Fourier transformation:

$$\begin{array}{l} U_i = \frac{1}{\sqrt{N}} \sum\limits_k e^{ikR_i} U_k \\ p_i = \frac{1}{\sqrt{N}} \sum\limits_k e^{ikR_i} p_k \end{array},$$

which reduces the Hamiltonian to

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_k u_k^\alpha c_{\alpha\beta} u_{-k}^\beta + E_0.$$

Where we defined

$$C_{\alpha\beta}(k) = \sum_{R \neq 0} \frac{\partial^2 V}{\partial R_i \partial R_j}(1 - e^{ikR}).$$

$C_{\alpha\beta}(k)$ has several important properties $C_{\alpha\beta}(k)^\dagger = C_{\alpha\beta}(-k)$. If the interaction ν is short ranged $C_{\alpha\beta}(k) \sim K^2$ as $K \to 0$. For each k it as the eigenvalues and eigenvectors;

$$\sum_\beta C_{\alpha\beta}(k) \varepsilon_s^\beta(k) = m\omega_s^2(k) \varepsilon_s^\alpha(k), \quad s = 1, 2, 3$$

ω_s^2 are the classical frequencies of oscillation of the crystal. We will assume that $V(r) = V(-r)$ do that $\omega_k = \omega_{-k}$ and $\varepsilon_s(k)^\dagger = \varepsilon_s(-k)$. Defining normal coordinates $U_s(k)P_s(k)$ by

$$\begin{array}{l} u_k^\alpha = \sum\limits_s \varepsilon_s^\alpha(k) u_s(k) \\ p_k^\alpha = \sum\limits_s \varepsilon_s^\alpha(k) p_s^\alpha(k) \end{array},$$

we can rewrite the H as

$$H_0 = \sum_{k,s} \frac{1}{2m} p_{ks} p_{-ks} + m\omega_0^2(k) u_{ks} u_{-ks}. \tag{8}$$

By analogy with the harmonic oscillator (problem l A) where

$$H = \frac{p^2}{2m} + m\omega^2 x^2,$$

was diagonalized by defining $x = \sqrt{\frac{1}{2m\omega}}\left(a + a^\dagger\right);\ p = \sqrt{\frac{m\omega}{2}} i \left(a - a^\dagger\right)$ we define

$$\begin{array}{l} U_s = \sqrt{\frac{1}{2m\omega_{sk}}}\left(a_{ks} + a_{-ks}^\dagger\right) \\ p_s = \sqrt{\frac{m\omega_{ks}}{2}} i \left(a_{ks} - a_{-ks}^\dagger\right) \end{array}.$$

The operator $a_{ks}^\dagger$ meets an excitation (phonon) with momentum k; sincea_{-ks} also add momentum k by removing a phonon from the ground state $u_s^\dagger(k)$ adds momentum k , substitution in (8) yields:

$$H_0 = \sum_{k,s} \omega_{ks} \left(a_{ks}^\dagger a_{ks} + \frac{1}{2}\right)$$