The Superfluid phases of Helium 3

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Abstract

The BCS theory for spin singlet and triplet pairing states is used to study the phases of liquid Helium 3. Expressions for the spin susceptibility and specific heat are derived and compared with experiment.
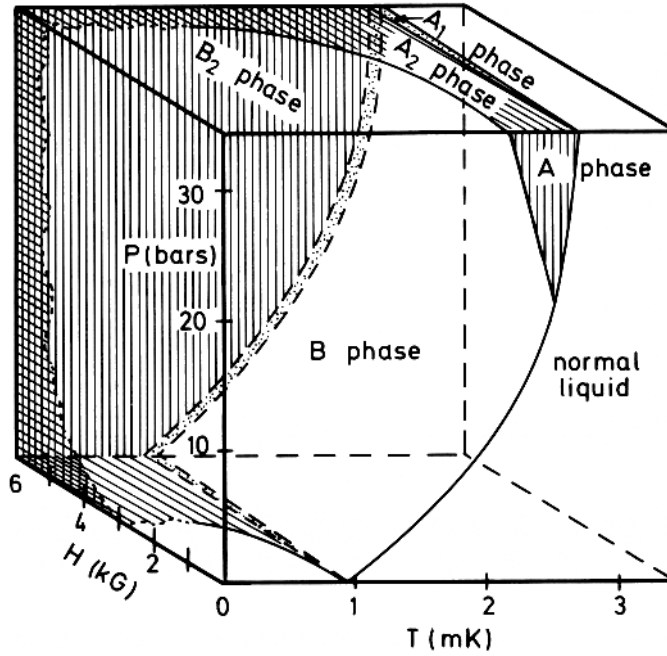
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Figure 1: Phase diagram of Helium 3. After [1]

1 Introduction

Helium 3 at low temperatures displays a wide variety of interesting features. Three distinct stable super-fluid phases of bulk Helium 3 have been identified; these are referred to as the A,B and A_1 phases. In zero magnetic field, only the A and B phases are stable. The phase diagram of Helium 3 is shown in Figure 1.

The mechanism of spin fluctuation exchange can lead to an attractive potential in Helium 3 and this in turn can lead to the phenomenon of Cooper pairing, He 3 being a fermionic system. Unlike the BCS ground state for normal superconductors where the relative angular momentum of the pairs is zero, in the case of Helium 3, Cooper pairing is likely to occur in higher angular momentum sites due to hard core repulsions. Such a state would have an anisotropic wavefunction and presumably anisotropic properties. Moreover since the He 3 atom is neutral, it does not show any anomalous electrical conduction properties like superconductivity, but it does show corresponding anomalous mass flow properties, namely superfluidity. The theory of anisotropic superfluidity, of which an account follows, has been developed in some depth and has been quiet successful in accounting for the properties of He 3 A and B. This is a rich and vast field. In the following, a rather abridged and introductory treatment of the theory has been presented leaving out such subjects as Ginzburg Landau theory, Fermi Liquid corrections, spin fluctuations, feedback effects and "strong coupling".

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2 BCS Theory at T = 0

Our first ansatz is a generalized form of the BCS ansatz on the nature of the ground state wavefunction for a sea of fermions.[1]

$$\psi = \prod_k{}' \prod_\alpha (u_{k\alpha\alpha} + \sum_\beta v_{k\alpha\beta} a_{k\alpha}^\dagger a_{-k\beta}^\dagger)|vac\rangle \tag{1}$$

The product over k is restricted to a half space to prevent double counting. In the case of s wave pairing, we have $v_{k\uparrow\downarrow} = -v_{k\downarrow\uparrow}$ and $v_{k\uparrow\uparrow} = v_{k\downarrow\downarrow} = 0$. To see that this leads to spin singlet pairing, consider the wavefunction

$$\begin{aligned}|\psi> &= v_{k\uparrow\downarrow}\left(|k,\uparrow;-k,\downarrow> - |k,\downarrow;-k,\uparrow>\right) \tag{2}\\ &= v_{k\uparrow\downarrow}\left(e^{ik.(r_1-r_2)} + e^{-ik.(r_1-r_2)}\right)(\uparrow\downarrow - \downarrow\uparrow) \tag{3}\end{aligned}$$

This ansatz is based on the phenomenon of Cooper pairing. In the case of superconductivity the pairing takes place in the s state. In the case of Helium, pairing occurs in higher angular momentum states leading to anisotropic properties. In the case of singlet pairing, one can also write down the ground state wavefunction as

$$\psi = \prod_{\text{all}k} \phi_k \tag{4}$$

where ϕ_k is the state

$$\phi_k = u_k|0,0\rangle_k + v_k|k\uparrow, -k\downarrow\rangle \tag{5}$$

where u_k and v_k are arbitrary complex parameters satisfying

$$|u_k|^2 + |v_k|^2 = 1, \qquad u_k = u_{-k} \qquad v_k = v_{-k} \tag{6}$$

The expectation value of the free energy is given by

$$\langle H - \mu N \rangle = \langle K - \mu N \rangle + \langle V \rangle \tag{7}$$

where μ is the fermi energy.

$$\langle K - \mu N \rangle = \sum_k \epsilon_k (n_{k\downarrow} + n_{k\uparrow}) \tag{8}$$

where ϵ_k is the kinetic energy minus the fermi energy, and

$$n_{k\uparrow} = a_{k\uparrow}^\dagger a_{k\uparrow} \tag{9}$$

$$n_{k\downarrow} = a_{k\downarrow}^\dagger a_{k\downarrow} \tag{10}$$

One can easily verify that

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$$\langle n_{k\uparrow}\rangle = \langle n_{k\downarrow}\rangle = |v_k|^2 \tag{11}$$

We assume after BCS [2], that the potential is of the form

$$
\begin{aligned}
V &= \frac{1}{2}\sum_{k,k'} V(k,k')[\langle a_{k'\uparrow}^\dagger a_{-k'\downarrow}^\dagger a_{-k\downarrow}a_{k\uparrow}\rangle \\
&\quad + \langle a_{k'\downarrow}^\dagger a_{-k'\uparrow}^\dagger a_{-k\uparrow}a_{k\downarrow}\rangle] \tag{12}
\end{aligned}
$$

$$\tag{13}$$

Consequently

$$\langle V\rangle = \sum_{k,k'} V_{k,k'}(u_k^* v_k u_{k'} v_{k'}^*) \tag{14}$$

We express the parameters u_k and v_k in terms of the single complex parameter Δ_k. Note that only the relative phase of u_k and v_k matters.

$$v_k \equiv \Delta_k / \left[|\Delta_k|^2 + (E_k + \epsilon_k)^2)\right]^{1/2} \tag{15}$$

$$u_k \equiv (E_k + \epsilon_k) / \left[|\Delta_k|^2 + (E_k + \epsilon_k)^2)\right]^{1/2} \tag{16}$$

where

$$E_k \equiv +(|\Delta_k|^2 + \epsilon_k^2)^{1/2} \tag{17}$$

The entropy may now be written down using the formula

$$S = \sum_k S_k \tag{18}$$

where S_k is given by the usual expression

$$S_k = -k_\beta \sum_n P_n ln P_n \tag{19}$$

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We then minimize the free energy (see [3] for details) with respect to the Δ_k's to obtain the gap equation at zero temperature.

$$\Delta_k = -\sum_{k'} V_{k,k'} F_{k'} \tag{20}$$

where $F_{k'} \equiv u_k^* v_k$.

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3   Excited States and BCS theory at Non Zero Temperature

The BCS ground state is the product of pair states, one state corresponding to each value of k. We wish to obtain the excited states of the system, ie states which are eigenstates of the BCS Hamiltonian with energies higher the ground state. We can intuitively guess that these should be product states as well, ie that the excited states of the BCS Hamiltonian can be obtained as the product states of excited and ground state pair states. The simplest such excited states are the ones where the state of occupation of a single pair is changed. For a given pair state, $\phi_k = (u_k|0,0\rangle_k + v_k|1,1\rangle_k)$ we can form two "broken pair" (BP) states which are the single occupancy states , $|k\uparrow\rangle$ and $|-k\downarrow\rangle$. The energy of this state can be calculated to be

$$E_{BP} = E_{GP} + E_k \tag{21}$$

We can also form an excited state by choosing an orthonormal pair state. One can show that the unique normalized state which is orthogonal to the ground state that can be constructed in this way is

$$\phi_{k(EP)} = \tilde{u}_k|0,0\rangle + \tilde{v}_k|1,1\rangle_k : \qquad \tilde{u}_k = v_k^*, \tilde{v}_k = -u_k^* \tag{22}$$

This state is called the "excited pair" (EP) state and its energy is

$$E_{EP} = E_{GP} + 2E_k \tag{23}$$

At non zero temperatures too we obtain the gap equation by minimizing the free energy. The coefficients and the complex parameters introduced become temperature dependent. Thus the ground and excited states are no longer the same as in the T = 0 case.

We anticipate the result that the broken pair and excited pair states have energies $E_k(T)$ and $2E_K(T)$. We then make the ansatz that the probabilities of occurrence of the GP, BP and EP states are

$$P_{GP} = n^{-1} \tag{24}$$

$$P_{BP} = n^{-1}exp\left[-\beta E_k(T)\right] \tag{25}$$

$$P_{EP} = n^{-1}exp\left[-2\beta E_k(T)\right] \tag{26}$$

$$n \equiv 1 + exp\left[-2\beta E_k(T)\right] + exp\left[-\beta E_k(T)\right] \tag{27}$$

$$\beta = 1/k_B T \tag{28}$$

It is now easy to write down the expectation values of the Kinetic and Potential terms of the Hamiltonian. Here, we will merely state the famous BCS gap equation,

which is obtained by imposing the maximization of free energy condition as in the
T = 0 case.

$$\Delta_k(T) = -\sum_{k'} V((k, k')[\Delta_{k'}(T)/2E_{k'}(T)] \times \tanh{[\beta E_{k'}(T/2]} \qquad (29)$$

The properties to the solutions of the gap equation are extensively studied in [4].

Specific Heat   The specific heat is obtained from the entropy by differentiation.
We find

$$C_v \equiv T(dS/dT) = \sum_k (k_B \frac{1}{2}\beta^2) \left[E_k + \beta(dE_k/d\beta)\right] \times (E_k sech^2(\beta E_k/2)) \qquad (30)$$

Above T_c, this expression reduces to the well known expression for the specific
heat of a BCS superconductor with a jump in C_v across T_c. It falls sharply as T
goes to zero owing to the exponential fall of the $sech^2 \beta E_k/2$. In the BCS case,
Δ is constant, whereas the gap Δ_n may have nodes in the case of an anisotropic
superfluid. The specific heat jum across T_c defined to be the difference between C_v
just below and above T_c is given by

$$\Delta C_v = \frac{1}{2} k_B \beta_c^3 \sum_k \left[E_k(dE_k/d\beta)\right] sech^2(\frac{1}{2}\beta_c E_k) \qquad (31)$$

Spin Susceptibility   The spin susceptibility of an isotropic superfluid is strongly
reduced with spin singlet pairing. To see why this is so, consider the fermi surface
of the superfluid in the singlet state. The up-spin and down-spin surfaces are split
up as seen in Fig.2. Thus the up-spin states in the shaded region are excluded from
forming Cooper pairs, though there are empty down spin states. Thus the system
has the choice between retaining its polarization and losing condensate energy or
reducing the polarization and increasing its condensation energy. It turns out that
it is energetically favorable to do the latter.

Let us now consider the effect quantitatively. The energies of the single particle
states $k \uparrow$ and $k \downarrow$ are shifted :

$$\epsilon_{k\uparrow} = \epsilon_k - 1/2\mu H \qquad \epsilon_{k\downarrow} = \epsilon_k + 1/2\mu H \qquad (\mu \equiv \gamma\hbar) \qquad (32)$$

Thus to first order in H, the energies of the GP and the EP states are not affected
whereas the energy of the BP states are. The contributions to the magnetization
too arise only from the BP states. The magnetization is given by

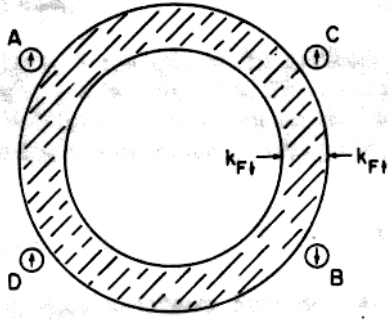$$M = \frac{1}{2}\mu \sum_k [P(1, 0) - P(0, 1)] \qquad (33)$$

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Figure 2: Effect of a magnetic field on the formation of Cooper pairs. Particles A and B cannot form a pair, but particles C and D can. After Leggett [3]

The probabilities of all the states are changed due to the energy change of the BP states. Keeping this in mind, the evaluation of M gives

$$M \approx \frac{1}{4}\mu^2 H \sum_k \frac{1}{2}\beta sech^2(\frac{1}{2}\beta E_K) \tag{34}$$

Thus the susceptibility χ neglecting Fermi liquid effects is

$$\chi_0 = \frac{1}{4}\mu^2 (dn/d\epsilon)Y(T) \tag{35}$$

where Y(T) is the Yosida function

$$Y(T) \equiv \int (d\omega/4\pi)Y(n:T) \tag{36}$$

and $Y(n:T) \equiv \int d\epsilon_k(1/2\beta sech^2(1/2)\beta E_k)$.

4   Spin Triplet Pairing

In this section we will try to solve the BCS problem for the spin triplet case. There is no obvious way to carry over our results from the spin singlet case except in the simple case of ESP states. ESP states are defined as triplet states whose component in the m = 0 spin state is zero at all points in space in some frame . To elaborate, the pair wave function, (also called the pseudomolecular wavefunction in literature) can be written as

$$\phi(r_1 - r_2, \sigma_1\sigma_2) \quad = \quad \phi_{\uparrow\uparrow}(r_1 - r_2)|\uparrow\uparrow\rangle + \phi_{\uparrow\downarrow}(r_1 - r_2)|\uparrow\downarrow + \downarrow\uparrow\rangle + \phi_{\downarrow\downarrow}(r_1 - r_2)|\downarrow\downarrow\rangle$$

Thus ESP states are states where by a suitable choice of axes, we can ensure that $\phi_{\uparrow\downarrow}(r_1 - r_2)$ is zero everywhere in space. In the ESP case, the ground state

wavefunction can be written as a product of the wave functions for the up and the down states

$$\psi = \psi_\uparrow \psi_\downarrow \equiv \prod_{all\ k} (u_{k\uparrow} + v_{k\uparrow} a^\dagger_{k\uparrow} a^\dagger_{-k\uparrow}) \times (u_{k\downarrow} + v_{k\downarrow} a^\dagger_{k\downarrow} a^\dagger_{-k\downarrow}) |vac\rangle \qquad (37)$$

Thus we can define two independent sets of parameters for the up and down states and the problem splits into two independent problems. The free energy of the system can be written as the sum

$$F(\Delta_{k\uparrow}, \Delta_{k\downarrow}) = \frac{1}{2} \sum_k [f(\Delta_{k\uparrow}) + f(\Delta_{k\downarrow})] \qquad (38)$$

the factor of half arising because of the fact that to avoid double counting we need to divide the equations [8] and [13] by a factor of two.

We thus get two independent gap equations, each of the same form as the singlet case. Thus all the results of the singlet discussion carry over to the present case if we make the replacement in all formulas

$$\sum_k g(E_k) \to \sum_k \frac{1}{2} g(E_{k\uparrow}) + g(E_{k\downarrow}) \qquad (39)$$

where $g(E_k)$ is any scalar thermodynamic function such as the specific heat for the singlet case. The only exception is the spin susceptibility. The intuitive argument used in the singlet case fails here as here we wish to pair particles of the same spin which have identical fermi surfaces. In the singlet case, we wanted to pair particles of opposite spins whose fermi surfaces were different. In other words, if we wish to pair a particle in the state $k \uparrow$ with one in $-k \uparrow$, this is possible even in the presence of a magnetic field. (See Fig. 2.) Thus formation of the superfuluid does not prevent the system from polarizing and hence the spin susceptibility of an ESP state should be identical to the normal phase. This is an important clue to determine from experiments whether a given phase corresponds to ESP states or not.

5   General Triplet States

We will first undertake the exercise of describing an ESP state, when we transform the spin axes so that the pair state wave function no longer has $\psi_{\uparrow\downarrow} = 0$ with respect to the new axes. For the subset of ESP states in which $\phi_{\uparrow\downarrow} = ex(i\chi)\phi_{\downarrow\downarrow}(r_1 - r_2)$ where χ is a real constant, one can ensure by a suitable transformation of the axes that $\phi_{\uparrow\downarrow} = 0$ in the new axes. The pair state wave function is then very similar to Eqn[2]. The subsequent treatment goes through in exact analogy with the spin singlet case. To obtain a description of the system which can be used to describe an ESP state in arbitrary frame, we treat the quantities $\Delta_{k\alpha\beta}$ as the components of a two by two matrix. Now all scalar quantities can be obtained by the replacement

$$\sum_k f(\Delta_k) \to \frac{1}{2} Tr \hat{f}(\hat{\Delta}_k) \qquad (40)$$

Now, given a non ESP triplet state, for a given value of k, it is always possible by a suitable transformation of axes to make the pair state ESP. Since the potential only scatters $S_z = +1$ states into $S_z = +1$ states, the description developed above is quite general and can be used even for non ESP states. In fact one can see that since the contribution of each k term to the free energy is independent, we can choose the spin axes appropriately for each k, and then transform the axes for each k so that the final reference frame is the same for all k. A more rigorous treatment for general triplet states can be found in [5]

The vector notation   Let $\hat{Q} \equiv Q_{\alpha\beta}$ be any symmetric function (such as $\hat{F}_k$, $\hat{\Delta}_k$) obtained in the spin triplet case on carrying out the replacement of the gap parameter of the singlet case by the gap matrix. From the elements of $\hat{Q}$ we can form a complex vector Q by the prescription

$$Q_i \equiv -\frac{1}{2} i \sum_{\alpha\beta} (\sigma_2 \sigma_i)_{\alpha\beta} Q_{\alpha\beta} \qquad (41)$$

where the σ_i are the Pauli sigma matrices.Inversion gives

$$\hat{Q} = \begin{pmatrix} -Q_x + iQ_y & Q_z \\ Q_z & Q_x + iQ_y \end{pmatrix} \qquad (42)$$

We denote the transform of the matrix $\hat{\Delta}_k$ by Eq. (41) as the vector $d(n)$. We define a unitary state as one which satisfies the criterion

$$\hat{\Delta}_k . \hat{\Delta}_k^\dagger = c(n) \hat{1} \qquad (43)$$

where $\hat{1}$ is the identity matrix. We list a few of the properties of the vector $d(n)$ For unitary states, the vector $d(n)$ turns out to be real. Further in an unitary state, the pairs at any given point on the Fermi surface condense into a spin state which is an eigenstate of the spin projection along the axis along which $d(n)$ points. The magnitude of $d(n)$ is a measure of the total amplitude of condensation of the Cooper pairs at point n on the Fermi surface, irrespective of spin. For an ESP state in the proper axis, the vector d(n) always lies in the xy plane for all n.

Thermodynamic properties of Triplet States   As discussed previously, thermodynamic quantities such as the specific heat which do not explicitly involve spin coordinates can be obtained by a simple generalization of the formulas for the singlet case. We just make the substitution

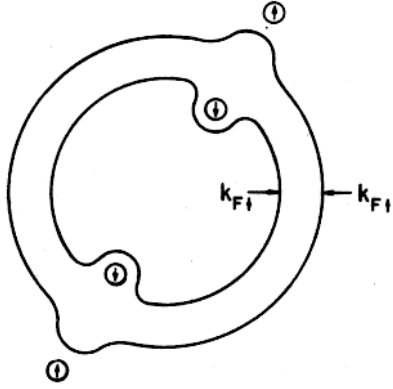$$\sum_k \to \sum_k \frac{1}{2} Tr \qquad (44)$$

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Figure 3: Differential polarization of the Fermi surface. After [3]

The spin dependent properties such as the spin susceptibility are harder to calculate. Assume that the Cooper pairs have a definite spin configuration independent of the external magnetic field. Define the differential susceptibility, i.e the quantity $\chi(n)$ given by

$$S(n)^i = \chi(n)H^i, S(n)^i \equiv \sum_{|k|} \hbar \sigma_k^i \tag{45}$$

The magnetic susceptibility is related to the differential susceptibility by

$$\chi = \int (d\Omega/4\pi)\chi(n) \tag{46}$$

Suppose in the ESP axes for the point n, the field H is along the z axis. Then we can apply the argument we applied in the ESP triplet case for the differential polarization of the Fermi surface as in Fig 3. As a consequence, the susceptibility with respect to the ESP z axis is equal to the normal value χ_n . On the other hand, if the field is along the direction of d(n) for an unitary state, in which case only $\Delta_{\uparrow\downarrow}$ is nonzero, then we can clearly apply the arguments used in the case of singlet pairing and obtain

$$\chi_\perp(n) = \chi_n Y(n : T) \tag{47}$$

where $Y(n : T)$ is the Yosida function. One can generalize the above results to obtain the differential susceptibility tensor,

$$\chi_{ij}(N) = \chi_n \times \left[\delta_{ij} - [1 - Y(n : T)][d_i^*(N)d_j(n)/|d(n)|^2]\right] \tag{48}$$

6   Comparison with experiments

In this section we try to account for the experimental data available on $^3He - A$ and B. We will look at the experimental data for the phase diagram, specific heat and
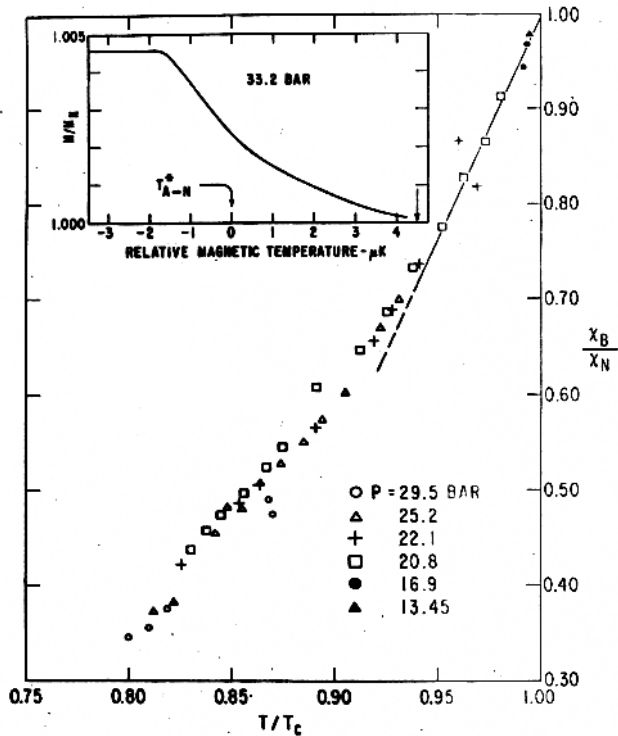
Figure 4: Magnetic Susceptibility in Helium 3 -B relative to the normal susceptibility χ_n. After [6]

the spin susceptibility [6]. The spin susceptibility of $^3He - A$ is pretty close to that of the normal fluid and is temperature independent. Since the spin susceptibility of both the spin singlet and the non-ESP triplet states is lower than the normal, $^3He - A$ is an ESP state, if it is a triplet state. As for $^3He - B$, its susceptibility is lower than the normal, but remains non zero as the temperature tends to zero (Fig4). This thus rules out both spin singlet and ESP triplet pairing. This leads us to conclude that both the A and the B phases correspond to triplet pairing, the A being ESP and the B phase non ESP.

The jump in the specific heat across the A-N and the B-N transition is quite large and then falls rapidly in both cases as the temperature is reduced. This is in agreement with theory.However the actual magnitude of the jump at T_c which according to the results presented should not be more than 1.42 is actually between 1.6 and 1.9. See Fig5

7   Conclusion

We developed the BCS theory for spin singlet and triplet states. We used it to obtain expressions for the spin susceptibility and specific heat of these states. These
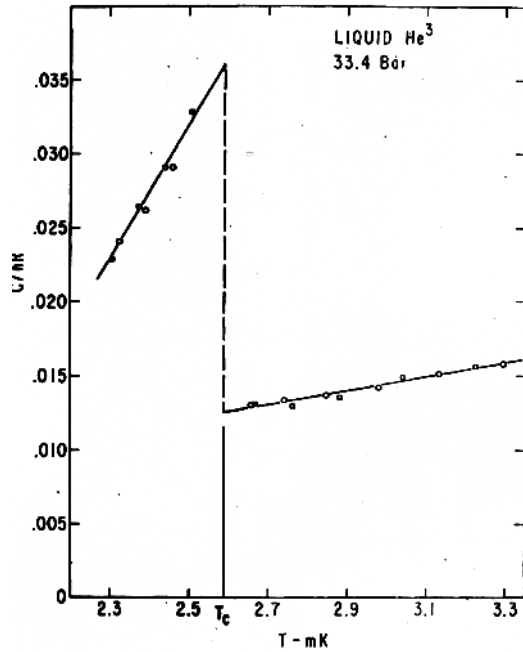
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Figure 5: Specific Heat of Helium 3 near the second order transition. [6]

were compared with the experimental values of these quantities and this comparison led us to identify the He 3 -A state as a ESP triplet state and the B state as being a non ESP triplet state.

References

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