OCCUPATION NUMBER REPRESENTATION FOR BOSONS AND SUPERFLUIDITY

SUMMARY OF THE SEMINAR TALK
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Contents

1. Motivation

When superfluidity in ^{4}He was discovered in 1938 no one was able to explain it. The phenomenon of zero viscosity within a liquid seemed to not fit to the classical knowledge of fluids. How could a liquid leak through solid surfaces such as ceramic? Why is a superfluid liquid able to climb up the walls of its container? And how does the so called frictionless fountain with a superfluid work? New theories were needed to explain the phenomenon of superfluidity in ^{4}He.

2. History

The observation of liquid ^{4}He began in 1908 with its first liquefaction. Thirty years passed until P. Kapitza discovered the superfluidity of ^{4}He and published his results in Nature in 1938. In the same edition similar results were published by J.F. Allen and A.D. Misener. But it was P. Kapitza who finally got the Nobel Prize 40 years later in 1978 for the discovery of superfluidity. Meanwhile, the Bose-Einstein condensate was predicted in 1925 by S. Bose and A. Einstein, and P.A.M. Dirac wrote his paper *The Quantum Theory of the Emission and Absorption of Radiation* in 1927. The latter was the origin of the second quantization. In the years after 1938, theorists where working on explanations for Kapitza's discovery. The first explanation then was developed by L.D. Landau considering ^{4}He as a quantum liquid in 1941. He therefore got the Nobel Prize in 1962. In between, a microscopic theory of superfluidity was developed by Bogoliubov in 1947. The fact that superfluidity is not limited to ^{4}He but also exists in ^{3}He was experimentally proven in 1971. In contrast to superfluidity, which was discovered first and then explained, the Bose-Einstein condensate was first theoretically predicted and not before 70 years later such condensates were experimentally realized in ultracold gases in 1995.

3. Introduction: Superfluidity by Landau

The phenomenon of superfluidity was first theoretically explained by Lew Dawidowitsch Landau. His theory of ^{4}He as a quantum liquid can be used as an introduction.

Landau's theory is based on a thought experiment which considers liquid ^{4}He below the critical temperature T_C in a tube. It is assumed that the liquid totally is in its ground state. This set up now is observed from two different point of views, the laboratory system K and the rest frame of liquid K_0.
The two systems are connected with a Galilean transformation. For the momentum P and energy E we get:

$$\vec{P} = \vec{P}_0 - M\vec{v}$$
$$E = \frac{P^2}{2M} = \frac{P_0^2}{2M} - \vec{P}_0 * \vec{v} + \frac{Mv^2}{2}$$

The ground state is

$$E_0 = E_0^g = 0 \qquad\qquad \vec{P}_0 = 0$$
$$E = E^g = E_0^g + \frac{Mv^2}{2} \qquad\qquad \vec{P} = -M\vec{v}$$

In the rest frame of the liquid flow resistance occurs when kinetic energy from the walls of the tube is transferred into the liquid. That means that so called quasiparticles have to be excited from the ground state. If such a quasiparticle with the momentum $\vec{k}$ and energy $\omega_{\vec{k}}$ is excited, the energy and momentum change to

$$E_0 = E_0^g + \omega_{\vec{k}} \qquad\qquad \vec{P}_0 = \vec{k}$$

$$E = E_0^g + \omega_{\vec{k}} - \vec{k} * \vec{v} + \frac{Mv^2}{2} \qquad\qquad \vec{P} = \vec{k} - M\vec{v}$$

Kinetic energy is transferred into the liquid, if the excitation energy in K is negative.

$$\Delta E = \omega_{\vec{k}} - \vec{k}\vec{v} < 0$$

The minimal excitation energy is given if $\vec{v} \parallel \vec{k}$.

$$min\Delta E = \omega_{\vec{k}} - kv < 0$$

From the minimal excitation energy we follow that feasible excitations are equal to a higher velocity than the critical velocity v_c.

$$v > v_c = \frac{\omega_{\vec{k}}}{k}$$

For $v < v_c$ the liquid flows without any friction, it is superfluid.

4. Second Quantization for Bosons

The phenomenon of superfluidity shall now be explained with a more general and quantum mechanically correct method. To do so, a mathematical method is needed that describes many body system with the particle number $N \gg 1$. Further on, the total particle number of the system does not have to be conserved due to the fact that interacting systems shall be described. The basic idea for that method is to let the occupation number be variable instead of position and spin. This requires a transformation of states and operators in the representation with occupation numbers that will result in the so called equivalent second quantization.

4.1. **Identical Particles.**

We start with a system of N identical particles. One way to describe the state is the wave function $\Psi(x_1, x_2, ..., x_N)$ where the variable x_i of the i-th particle represents its position and spin. To be identical now means that a permutation P of particles cannot be measured. For N particles there are N! possibilities to sort the particles, these shall from now on be the elements of the group S_N. In nature, there are two possible linear combinations of the wave functions, on the one hand the total symmetric wave function Ψ_S on the other the total antisymmetric one Ψ_a.

$$\Psi_S = \frac{1}{\sqrt{N!}} \sum_{P_N \in S_N} \hat{P}\Psi \qquad\qquad \Psi_a = \frac{1}{\sqrt{N!}} \sum_{P_N \in S_N} sgn(P)\hat{P}\Psi$$

Whereas exchanging two particles in the symmetric wave function does not change the wave function. In contrast to that, exchanging two particles in the antisymmetric wave function results in a minus sign in front of the wave function. The symmetric system is described by the Bose-Einstein statistics and is valid for bosons with an integer spin such as photons and ^{4}He. The antisymmetric wave function is also called the Fermi-Dirac statistics and describes particles with a half-integer spin such as electrons or ^{3}He. The connection between the statistics and the spins of the particles is given by the Relativistic Spin Statistic Theorem by W. Pauli.
A possible symmetric or antisymmetric can now be described in the following way. An orthonormal basis for a single particle can be written as $|i\rangle$ $i = 1, 2, 3, ...$ with $\langle i|j\rangle = \delta_{ij}$. The orthonormal basis for N particles would then be the tensor product $|i_1, ..., i_k, ..., i_N\rangle :=$ $|i_1\rangle \otimes ... \otimes |i_k\rangle \otimes ... \otimes |i_N\rangle$ where the particle k occupies the state $|i_k\rangle$. Applying the symmetrizing operator $\hat{S}_\pm = \frac{1}{\sqrt{N!}} \sum_{P\in S_N} (\pm)^P \hat{P}$ to the (anti)symmetric wave function yields in (anti)symmetric basis states.

$$\hat{S}_\pm|i_1, ..., i_k, ..., i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{P\in S_N} (\pm)^P \hat{P}|i_1, ..., i_k, ..., i_N\rangle$$

4.2. **Occupation Number as Basis.**

The defined basis states are neither normalized nor linear independent. For bosons, the sum over all possible permutations results in a sum with equivalent terms. The antisymmetric case for fermions shall be omitted further on. At first, normalization of the basis states can be reached by using the appropriate normalization factor. Secondly, linear independence is reached by using the occupation number representation where $n_i = 0, 1, 2, ...$ is the multiplicity of state $|i\rangle$.

$$|n_1, n_2, ...\rangle = \frac{1}{\sqrt{n_1!n_2!...}} \hat{S}_+|i_1, i_2, ..., i_N\rangle$$

This occupation number basis is an orthonormal basis for the Hilbert space H_N for $N = \sum_i n_i$ identical particles. The Hilbert spaces can be combined in the so called Fock space.

$$H = H_0 \oplus H_1 \oplus H_2 \oplus H_3 \oplus ... = \bigoplus_{N=0}^{\infty} H_N$$

The Hilbert space H_0 only contains one element, the vacuum.

$$|0\rangle = |0, 0, 0, ...\rangle$$

4.3. **Ladder Operators.**

In order to describe systems with a variable number of particles, you need to be able to navigate through the Fock space, from one Hilbert space to another. For that ladder operators can be defined. The creation operator $\hat{a}_i^\dagger$ increases the occupation number n_i by one, whereas the annihilation operator $\hat{a}_i$ decreases the occupation number n_i by one. The navigation through the Fock space with these ladder operators can be illustrated as it is done in Figure 1.

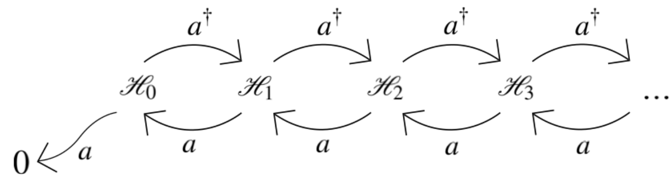

FIGURE 1. Navigation through Fock Space[1]

The creation and annihilation operator is defined as follows

$$\hat{a}_i^\dagger |..., n_i, ...\rangle := \sqrt{n_i + 1}|..., n_i + 1, ...\rangle$$

$$\hat{a}_i |..., n_i, ...\rangle = \begin{cases} \sqrt{n_i}|..., n_i - 1, ...\rangle & \text{if } n_i \geqq 1, \\ 0 & \text{if } n_i = 0. \end{cases}$$

The commutation relations can be calculated directly from the definitions of the operators.

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0 \qquad\qquad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$$

As a result, the occupation number states can now be written with the ladder operators starting from the vacuum state.

$$|n_1, n_2, ...\rangle = \frac{1}{\sqrt{n_1! n_2! ...}} (\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} ... |0\rangle$$

Last but not least, using the ladder operators you can also define the particle number operator $\hat{n}_i$ and the total particle number operator $\hat{N}_i$.

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i \qquad\qquad \hat{n}_i |..., n_i, ...\rangle = n_i |..., n_i, ...\rangle$$

$$\hat{N} = \sum_i = \hat{n}_i \qquad\qquad \hat{N}|n_1, n_2, ...\rangle = \left(\sum_i \hat{n}_i\right)|n_1, n_2, ...\rangle = N|n_1, n_2, ...\rangle$$

4.4. **Operators in Occupation Number Representation.**

The aim is not only to rewrite states in the occupation number representation but also the Hamiltonians. Therefore, operators also have to be rewritten so that they operate on occupation number states. The derivation for the one particle operator shall be done explicitly while giving just the result for a two particle operator.

The one particle operator for N particles can be written as a sum over all one particle operators for each particle α.

$$T = \sum_{\alpha=1}^{N} t_\alpha$$

The matrix elements of the one particle operator for a single particle can be used to rewrite T in the following way.

$$t_{ij} = \langle i|t|j\rangle$$

$$\Rightarrow t = \sum_{ij} |i\rangle\langle i|t|j\rangle\langle j| = \sum_{ij} t_{ij}|i\rangle\langle j|$$

$$\Rightarrow T = \sum_{ij} t_{ij} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha$$

In order to rewrite T with the ladder operators we need to understand its impact on a state.
First case $i \neq j$:

$$\begin{aligned}
\sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha |..., n_i, ..., n_j, ...\rangle &= \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha \hat{S}_+ |i_1, i_2, ..., i_N\rangle \frac{1}{\sqrt{n_1! n_2! ...}} \\
&= \hat{S}_+ \frac{1}{\sqrt{n_1! ... n_i! ... n_j! ...}} \sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha |i_1, ..., i_N\rangle \\
&= \hat{S}_+ \frac{1}{\sqrt{n_1! n_2! ... (n_i+1)! ... (n_j-1)!}} \frac{\sqrt{n_i+1}}{\sqrt{n_j}} n_j |\tilde{1}_1, \tilde{i}_2, ..., \tilde{i}_N\rangle \\
&= n_j \frac{\sqrt{n_i+1}}{\sqrt{n_j}} |..., n_i+1, ... n_j-1, ...\rangle = \hat{a}_i^\dagger \hat{a}_j |..., n_i, ..., n_j, ...\rangle := (I)
\end{aligned}$$

Second case $i = j$:

$$(I) = \hat{n}_i |..., n_i, ...\rangle = \hat{a}_i^\dagger \hat{a}_i |..., n_i, ...\rangle := (II)$$

For every i,j the operator can be rewritten in occupation number representation:

$$\sum_{\alpha=1}^{N} |i\rangle_\alpha \langle j|_\alpha = \hat{a}_i^\dagger \hat{a}_j$$

The final result for the one particle operator T then is:

$$T = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j$$

The two or even more particle operator can be calculated as well. The Hamiltonian in the occupation number representation now reads

$$\hat{H} = \sum_{ij} H_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{i,j,k,m} v_{ijkm} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k + ...$$

$$v_{ijkm} = \int dx_\alpha dx_\beta \Phi_i * (x_\alpha) \Phi_j^*(x_\beta) v(x_\alpha, x_\beta) \Phi_k(x_\alpha) \Phi_m(x_\beta)$$

4.5. **Field Operators.**

The transformation of states and operators into the occupation number representation is basically finished. As a last step, field operators shall be introduced which allow a even more compact writing. The representation with the field operators is totally equivalent to the one with the former ladder operators.
The field operators are defined analogously to the ladder operators:

$$\hat{\Psi}(\vec{r}) = \sum_i \Phi_i(\vec{r})\hat{a}_i \qquad [\hat{\Psi}(\vec{r}), \hat{\Psi}(\vec{r}')] = [\hat{\Psi}^\dagger(\vec{r}), \hat{\Psi}^\dagger(\vec{r}')] = 0$$

$$\hat{\Psi}^\dagger(\vec{r}) = \sum_i \Phi_i(\vec{r})\hat{a}_i^\dagger \qquad [\hat{\Psi}(\vec{r}), \hat{\Psi}^\dagger(\vec{r}')] = \delta(\vec{r} - \vec{r}')$$

The operator $\hat{\Psi}^\dagger$ creates a particle in the position eigenstate, whereas $\hat{\Psi}$ annihilates a particle in the position eigenstate. The general one and two particle operator are:

$$\hat{T}^{(1)} = \int \hat{\Psi}^\dagger(\vec{r})t^(1)\hat{\Psi}(\vec{r})d\vec{r}$$

$$\hat{T}^{(2)} = \frac{1}{2}\iint \hat{\Psi}^\dagger(\vec{r})\hat{\Psi}^\dagger(\vec{r}')t^(2)\hat{\Psi}(\vec{r}')\hat{\Psi}(\vec{r})d\vec{r}d\vec{r}'$$

For example, the Hamiltonian can now be written with the field operators.

$$\hat{H} = \int d^3r\hat{\Psi}(\vec{r})\left(-\frac{\hbar^2}{2m}\Delta + U(\vec{r})\right)\hat{\Psi}(\vec{r}) + \frac{1}{2}\int d^3rd^3r'\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}^\dagger(\vec{r}')V(\vec{r},\vec{r}')\hat{\Psi}(\vec{r}')\hat{\Psi}(\vec{r})$$

With the representation along field operators it is obvious why the occupation number representation yields in the equivalently called second quantization. The quantization of the energy of particles can be interpreted as the first quantization, whereas the additional quantization of the fields then is named the second quantization.

5. Superfluidity

Finally, we can use the new mathematical method of the second quantization for bosons to describe an interacting system of many particles such as liquid ^{4}He. The fact that ^{4}He can be treated as having spin 0 allows this. With that, the characteristics of superfluidity below $T_\lambda = 2,18K$ shall be described mathematically.

5.1. **Weak Interaction.**

Here, we will assume liquid helium 4 to be a weakly interacting system. It actually is a strongly interacting system. But due to the fact that its derivation would be very complicated and cannot be solved analytically we assume weak interaction. Anyhow, the result will qualitatively be the same. The differences will be shown later on by comparing the theoretical results to experimental results. Start with the Hamiltonian from second quantization ($\hbar \equiv 1$).

$$\hat{H} = \sum_{\vec{k}} \frac{k^2}{2m} \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k},\vec{p},\vec{q}} V_{\vec{q}} \hat{a}^\dagger_{\vec{k}+\vec{q}} \hat{a}^\dagger_{\vec{p}-\vec{q}} \hat{a}_{\vec{p}} \hat{a}_{\vec{k}}$$

No interaction in the Bose liquid in its ground state would mean that the total particle number N equals the number of particles in the ground state n_0 and therefore the momentum is $\vec{k} = 0$. This then is the so called Bose-Einstein-condensate. In contrast to that, weak interaction shall now look like the following. The ground state with $\vec{k}$ is still occupied macroscopically so that the particle number in the ground state almost equals the total particle number.

$$n_0 \approx N$$

Under the assumption of weak interaction as described above the following approximations can be made always keeping in mind $n_0 \approx N$.

(1) neglect interaction of particles with $\vec{k} \neq 0$ with each other
(2) but consider interaction of particles with condensed particles
(3) and consider interaction of condensed particles with each other

$$\hat{H} = \sum_{\vec{k}} \frac{k^2}{m} \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} + \underbrace{\tfrac{1}{2V} V_0 \hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_0 \hat{a}_0}_{3} + \underbrace{\tfrac{1}{V} \sum_{\vec{k}\neq 0} (V_0 + V_{\vec{k}}) \hat{a}^\dagger_0 \hat{a}_0 \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} + \tfrac{1}{2V} \sum_{\vec{k}\neq 0} V_{\vec{k}} \left(\hat{a}^\dagger_{\vec{k}} \hat{a}^\dagger_{-\vec{k}} \hat{a}_0 \hat{a}_0 + \hat{a}^\dagger_0 \hat{a}^\dagger_0 \hat{a}_{\vec{k}} \hat{a}_{-\vec{k}} \right)}_{2} + \underbrace{O\left(\hat{a}^\dagger_{\vec{k}}\right)}_{1}$$

This Hamiltonian can now be simplified by using the following relations. First of all, it can be used that the creation and annihilation operator can be replaced by the number $\sqrt{n_0}$. This is because ± 1 can be neglected since n_0 is a high number.

$$\hat{a}_0 |n_0, ...\rangle = \sqrt{n_0} |n_0 - 1, ...\rangle \approx \sqrt{n_0} |n_0, ...\rangle$$

$$\hat{a}^\dagger_0 |n_0, ...\rangle = \sqrt{n_0 + 1} |n_0 + 1, ...\rangle \approx \sqrt{n_0} |n_0, ...\rangle$$

$$\Rightarrow \hat{a}_0 \approx \hat{a}^\dagger_0 \approx \sqrt{n_0}$$

Second, the total particle number $\hat{N}$ can be written as a sum of the number of particles in the ground state and the particle number of the excited particles.

$$\hat{N} = \hat{n_0} + \sum_{\vec{k}\neq 0} \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}}$$

In a third step we make use of Bogoliubov's approximation:

$$\sum_{\vec{k},\vec{k}'} \hat{a}^\dagger_{\vec{k}} \hat{a}_{\vec{k}} \hat{a}^\dagger_{\vec{k}'} \hat{a}_{\vec{k}'} \approx \left(\sum_{\vec{k}\neq 0} \hat{a}_{\vec{k}} \right)^2 \neq (N - n_0)^2 \to 0$$

At last, the Hamiltonian shall be diagonalized. This can be achieved with a Bogoliubov transformation: new operators $\hat{\alpha}$ are defined with commutation relations as for the ladder operators.

$$\hat{a}_{\vec{k}} = u_{\vec{a}}\hat{\alpha}_{\vec{k}} + v_{\vec{k}}\hat{\alpha}^{\dagger}_{-\vec{k}} \qquad [\hat{\alpha}_{\vec{k}}, \hat{\alpha}_{\vec{k}'}] = [\hat{\alpha}^{\dagger}_{\vec{k}}, \hat{a}^{\dagger}_{\vec{k}'}] = 0$$
$$\hat{a}^{\dagger}_{\vec{k}} = u_{\vec{k}}\hat{\alpha}^{\dagger}_{\vec{k}} + v_{\vec{k}}\hat{\alpha}_{-\vec{k}} \qquad [\hat{\alpha}_{\vec{k}}, \hat{\alpha}^{\dagger}_{\vec{k}}] = \delta_{\vec{k},\vec{k}'}$$

The newly introduced operators allow a diagonalized representation of the Hamiltonian hence the operators $\hat{\alpha}$ can be called quasiparticles. The liquid behaves as if the liquid would consist of these quasiparticles.

$$\hat{H} = \frac{N^2}{2V}V_0 - \frac{1}{2}\sum_{\vec{k}\neq 0}\left(\frac{k^2}{2m} + nV_{\vec{k}} - \omega_{\vec{k}}\right) + \sum_{\vec{k}\neq 0}\omega_{\vec{k}}\hat{\alpha}^{\dagger}_{\vec{k}}\hat{\alpha}_{\vec{k}} \qquad \omega_{\vec{k}} = \sqrt{\left(\frac{k^2}{2m}\right)^2 + \frac{nk^2V_{\vec{k}}}{m}}$$

The energy of the collective energy is given by the dispersion relation. This can be observed in two regimes.

(1) small $k = |\vec{k}| \Longrightarrow \omega \approx ck$
(2) large $k = |\vec{k}| \Longrightarrow \omega_{\vec{k}} = \frac{k^2}{2m} + nV_{\vec{k}}$

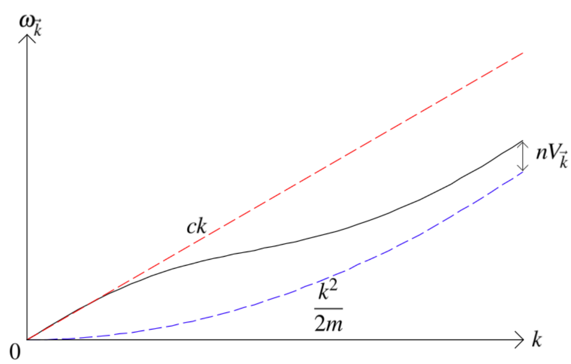

FIGURE 2. Dispersion relation of weakly interacting ^{4}He$^{(1)}$

5.2. **Real ^{4}He.**

As mentioned in the very beginning, liquid ^{4}He actually is not a system with weak but strong interaction. The correct result can not be calculated analytically but the differences can be shown by comparing the graph with an experimentally determined one (see Figure 3). In contrast to Figure 2 there is a minimum in the dispersion relation which results from the strong interaction.

Now, the connection to Landau's theory of ^{4}He as a quantum liquid from the very beginning can be made. The critical velocity calculated by Landau equals a tangent through zero on the curve. In case of weak and strong interaction this tangent can be drawn and yields in a critical velocity which is bigger than zero. For a velocity smaller than the

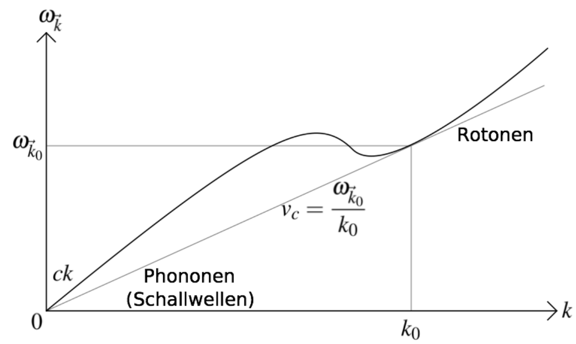

FIGURE 3. Experimentally determined dispersion relation of ^{4}He[(1)]

critical velocity a superfluid behaviour can be observed. In contrast to that, for an ideal (non-interacting) system the dispersion relation would be proportional to k^2 for all k (blue curve in Figure 2). In this case the tangent would result in $v_c = 0$ yielding in no superfluid regime.

6. Outlook

The superfluidity with the characteristic of zero viscosity in ^{4}He now is explained. In the paragraph about history it was mentioned that there is a superfluid regime in ^{3}He as well. The difference to the isotope ^{4}He is the fact that ^{3}He is a fermion and hence cannot be explained by using the assumption of a condensate in the ground state. The superfluidity of ^{3}He is more connected to the phenomenon of superconductivity. The strong interaction here leads to a polarisation of the spins of the atoms. Following Landau's theory, quasiparticles are formed with e new effective mass that interact weakly. On these quasiparticles the BCS (Bardeen, Cooper, Schrieffer) theory can then be applied.
The second quantization for fermions would yield in similar results but with anticommuting ladder operators and field operators.

7. References

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