Quantum Mechanical Aspects of Superfluidity

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Abstract: Under certain conditions ^{4}He undergoes a phase transition from a normal liquid to a superfluid state, with unique and remarkable characteristics. The statistical properties of an ideal Bose gas exhibit striking similarities to ^{4}He, suggesting that the observed phase transition is associated with the condensation of atoms into the lowest energy state. Since ^{4}He remains liquid at low temperatures, the normal modes of ^{4}He cannot be expected to be strictly harmonic and other elementary excitations beyond phonons, Landau's rotons, can be anticipated. In this work we discuss quantum aspects of the condensate and its wave function using the formalism of second quantization. The interacting system is studied developing the Hamiltonian in this formalism, finding the energy of the system in terms of the ground state energy plus excitations corresponding to the expected phonons. Introducing the theory of linear response and making use of the structure factor and general inequalities, again in the case of the weakly-interacting Bose gas, roton excitations are successfully described. Finally we briefly comment on the existence of quantized vortices.

I. INTRODUCTION

The statistical description of an ideal gas is rooted in the number of states associated with arranging n_i identical and indistinguishable particles into g_i energy levels, enabling the entropy of the system to be easily calculated through Boltzmann's relation. Employing the grand canonical formalism for bosons taking the energy spectrum as nearly continuous and using the calculation of the entropy of the system, the following expressions are derived [1]:

$$\frac{P}{kT} = -\frac{2\pi(2mkT)^{3/2}}{h^3}\int_0^\infty x^{1/2}\ln(1-ze^{-x})dx = \frac{1}{\lambda^3}g_{5/2}(z) \tag{1}$$

$$\frac{N-N_0}{V} = \frac{2\pi(2mkT)^{3/2}}{h^3}\int_0^\infty \frac{x^{1/2}dx}{z^{-1}e^x-1} = \frac{1}{\lambda^3}g_{3/2}(z) \tag{2}$$

where P is the pressure, V is the volume, T is the temperature, k is the Boltzmann constant, h is Planck's constant, $\lambda = h/(2\pi mkT)^{1/2}$ is the mean thermal wavelength and N and N_0 refer to the total number of particles and the number of particles in the ground state. In this expressions we make use of the Bose-Einstein functions $g_v(z) = z + z^2/2^v + z^3/3^v + \ldots$,where $z = e^{\beta\mu}$ is the fugacity, with μ the chemical potential . For an ideal Bose gas, the chemical potential must always be negative so the system's fugacity lies in the range $0 \le z \le 1$. Note also that $g_v(1) = \zeta(v)$, with ζ the Riemann zeta function; this upper bound for $g_v(z)$ together with (2) leads to:

$$N - N_0 = N_e \le V\frac{(2\pi mkT)^{3/2}}{h^3}\zeta\left(\frac{3}{2}\right) \tag{3}$$

with N_e the number of particles in the excited states, which approximately correspond to N unless $z \approx 1$. If the actual number of particles exceeds this limiting value, then it is natural that the excited states will accommodate as many particles as they can while the rest will be placed in mass into the ground state. This phenomenon is known as Bose-Einstein Condensation. If we hold N and V constant and vary T we find the following condition for the condensation [1]:

$$T < T_c = \frac{h^2}{2\pi mk}\left\{\frac{N}{V\zeta\left(\frac{3}{2}\right)}\right\}^{2/3} \tag{4}$$

For this T the system consists on a mixture of two phases, a normal phase N_e particles distributed over the excited states, and a condensed phase N_0 particles accumulated in the ground state; see Fig. 1.

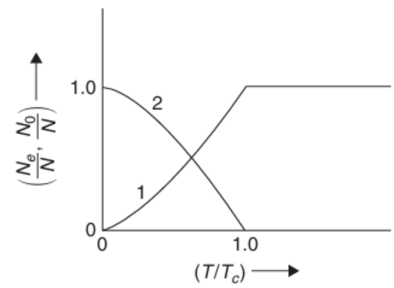

FIG. 1: Relative number of particles in the ground state "2" and in excited states "1" as a function of T.

Equation (1) allows us to examine in the $P(T)$ dependence of the Bose gas below, above and at the transition temperature again making use of the Bose-Einstein functions and their properties. With $P(T)$ it is possible to calculate the energy $U = \frac{3}{2}PV$, and from here, the constant volume heat capacity $C_v = (\frac{\partial U}{\partial T})_{N,V}$ of the Bose gas. The result is shown in Fig 2(a) and is strikingly "similar" to what is experimentally obtained for ^{4}He; see Fig. 2(b).

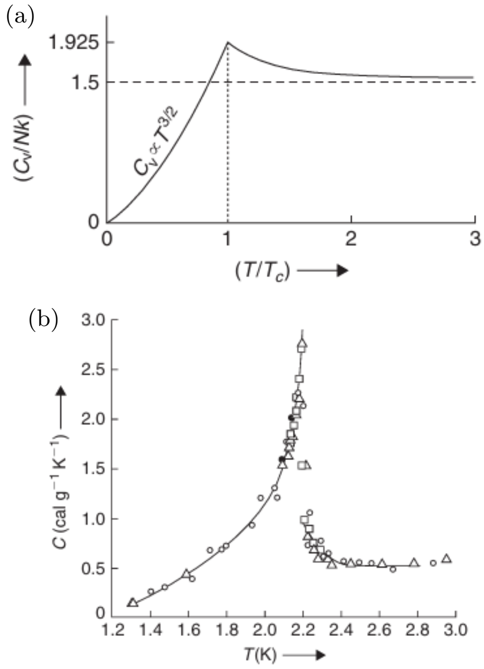

FIG. 2: (a) Theoretical specific heat of an ideal Bose gas as a function of T/T_c. (b) Experimental specific heat of liquid ^{4}He.

This similarity suggests that the phase transition observed in ^{4}He could be a manifestation of Bose-Einstein condensation with N_o particles identified as the superfluid component, and N_e number of particles associated with the normal fluid component. Support to this analogy comes from calculating the critical temperature of the condensation for an ideal Bose gas in the case of ^{4}He. We find 3,17K which is not far from the experimental phase transition temperature of superfluid helium $T_\lambda = 2,17K$. Note, however, that in ^{4}He, intermolecular interactions are important and its inclusion would improve the agreement. We now focus on studying superfluidity as a consequence of Bose Einstein condensation with special emphasis on the condensate and its excitations.

II. ELEMENTARY EXCITATIONS IN SUPERFLUID HELIUM

The problem of vibrational modes in a solid is usually approached very similarly to how Planck tackled the blackbody radiation problem. The system is considered as a set of harmonic oscillators. Considering its Hamiltonian in the harmonic approximation, we find that the system eigenstates have energy:

$$E\{n_i\} = \Phi_0 + \sum_i \left(n_i + \frac{1}{2}\right)\hbar\omega_i \tag{5}$$

where $\hbar = h/(2\pi)$ and $w_i (i = 1, 2, ..., 3N)$ are the characteristic frequencies of the normal modes of the system. The energy of the solid, beyond the minimum value Φ_0 can then be considered as originating from a set of 3N one-dimensional non-interacting harmonic oscillators. Quantum mechanically, these modes give rise to quanta, phonons, with n_i representing the occupation numbers of the single-particle energy levels. Our case, however, is different from this situation, ^{4}He remains liquid at low temperatures, hence no transverse modes are expected.

Additionally, the vibrational modes are not strictly harmonic, since the approximation of small amplitude should no longer be valid. Thus, in addition to phonons, other excitations are expected. To study the liquid excitations, we consider a flowing gas of phonons in mass motion. Since for phonons $\mu = 0$ the problem is not constrained by a fixed number N, our constraints are, a fixed momentum and a fixed total energy. In this case, the average occupation number for a phonon level is:

$$\langle n(\mathbf{p})\rangle = \frac{1}{\exp(\beta\epsilon + \vec{\gamma}\cdot\vec{\mathbf{p}}) - 1} \tag{6}$$

where $\vec{\gamma}$ is a Lagrange multiplier. Considering the drift velocity of the phonon gas $\vec{v}$, and that for phonons, $\epsilon = pc$ and $u \equiv d\epsilon/dp = c$, we find $\vec{\gamma} = -\beta\vec{v}$. With the average occupation number, we can calculate the total momentum of the phonon gas $\vec{P}$ and determine its inertial mass density as $\rho = \frac{P/v}{V}$. For $v << c$, which is generally valid and we obtain the phonon density normalized with the total density of the liquid:

$$\frac{\rho_{\rm ph}}{\rho_{\rm He}} = 1.22 \times 10^{-4} T^4 \tag{7}$$

At $T = 0,3K$ the value of this fraction is 9.9×10^{-7}. At this temperature, phonons are the only excitations to consider in ^{4}He. The calculated density can thus be associated with the density ρ_n of what we call the normal component of the liquid. At $T = 0K$ there are no excitations, $\rho_n = 0$ and the entire fluid is in the superfluid phase. At higher temperatures, we have $\rho_s = \rho_{He} - \rho_n$. At $T = T_\lambda$, $\rho_n = \rho_{He}$ and $\rho_s = 0$. For $T > T_c$ the liquid behaves completely as a normal fluid.

Experimentally, the energy-momentum relation $\epsilon(p)$ was measured by Yarnell (1959) using neutron scattering; the result at $T = 1,1K$ is shown in Fig.3.

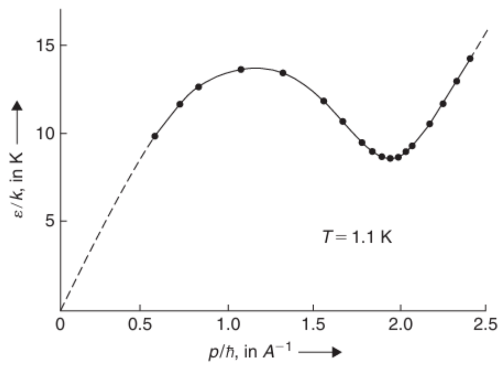

FIG. 3: Energy spectrum of elementary excitations in superfluid helium at $T = 1,1K$.

For low momentum, the primary excitations correspond to phonons $\epsilon = pc$, with $c = (239 \pm 5)m/s$, which is close to the measured speed of sound $238m/s$. There is a maximum followed by a minimum at larger q, corresponding to the other type of excitations. In the neighbourhood of the minimum, $\epsilon(p) = \Delta + \frac{(p-p_0)^2}{2\mu}$, with Δ, p_0, and μ constants, resembling the bosonic excitation that Landau called rotons.

III. QUANTUM MECHANICS OF BOSE-EINSTEIN CONDENSATE

When studying interacting quantum systems with many particles, the formalism of second quantization is very useful. This is based on the occupation number of each single-particle state, constructing the Fock space as the direct summation of the associated Hilbert spaces with different particle numbers. Field operators $\psi(\vec{r})$ and $\psi^\dagger(\vec{r})$ act on the Hilbert space by annihilating or creating a particle at position $\vec{r}$, the particle number operator is then defined as $\hat{N} \equiv \int \psi^\dagger(\vec{r})\psi(\vec{r})d\vec{r}$. Introducing a complete orthonormal set of single-particle wave-functions $u_\alpha(\vec{r})$ we can expand the field operators in terms of this basis to obtain the useful operators a_α and $a_\alpha^\dagger$. This operators act on the elements of the Fock space annihilating and creating a particle in the single-particle state α with the number operator now being $\hat{N} = \sum_\alpha a_\alpha^\dagger a_\alpha$. We now introduce the one-body density matrix:

$$n^{(1)}(\vec{r}, \vec{r'}) = \langle \hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r'})\rangle \tag{8}$$

This hermitian matrix encodes information on important physical observables. By setting $\vec{r} = \vec{r'}$ one finds the diagonal density of the system. For temperatures above the condensation temperature, $n^{(1)}(\vec{r}, \vec{r'})$ vanishes as the distance $|\vec{r} - \vec{r'}|$ increases. In contrast, for $T < T_c$ it does not vanish at large distances but approaches a finite value, $n_0 = N_0/V$. This behaviour, often referred to as off-diagonal long-range order, its strongly connected with the behaviour of its eigenvalues n_i, defined by the solution of the equation:

$$\int n^{(1)}(\vec{r}, \vec{r'})\phi_i(\vec{r'})d\vec{r'} = n_i\phi_i(\vec{r}) \tag{9}$$

The solutions provide a natural basis of orthonormal single-particle wave-functions $\int \phi_i^*\phi_j d\vec{r} = \delta_{ij}$, which are well defined not only for an ideal gas but also for interacting and non-uniform systems. We can show that plane waves are solutions for ϕ_i [2]. The eigenvalues n_i are the single-particle occupation numbers. Bose-Einstein condensation occurs when one of the states, the condensate $i = 0$ state, is occupied in a macroscopic way with $n_{i=0} \equiv N_0 \approx N$. The wave function relative to the macroscopic eigenvalue N_0 characterizes the wave function of the condensate and can be written using the single-particle state operators as:

$$\hat{\psi}(\vec{r}) = \phi_0(\vec{r})\hat{a}_0 + \sum_{i\neq 0}\phi_i(\vec{r})\hat{a}_i \tag{10}$$

At this point we introduce the Bogoliugov approximation, consisting in replacing the operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ with the c-number $\sqrt{N_0}$. This is a good approximation for describing the macroscopic phenomena associated with Bose-Einstein Condensation, where $N_0 = \langle \hat{a}_0^\dagger \hat{a}_0\rangle >> 1$. This approximation is equivalent to treating the macroscopic component $\phi_o\hat{a}_0$ of the field operator as a classical field. We can then write the condensate wave function as:

$$\psi = \psi_0 e^{iS(\vec{r})} \tag{11}$$

where ψ_0^2 is a measure of the condensed atoms and the phase $S(\vec{r})$ is a generalisation of $\vec{p}\cdot\vec{r}/\hbar$. The wave function of the condensate plays the role of an order parameter that vanishes over the transition temperature.

To study the energy of the Bose gas we must take into account the interactions between particles, which affect significantly the properties of the gas. In rarefied gases the range r_0 of interatomic forces is much smaller than the average distance between particles $r_0 < d$, with $d \approx n^{-1/3}$ fixed by the density $n = N/V$ of the gas. This allows considering only configurations involving pairs of interacting particles. In addition, the distance between two particles is always large enough to express all the interacting properties of the system in terms of the scattering amplitude a, which does not depend on specific details of two-body interaction. We now write the Hamiltonian of the system in terms of the creation and annihilation operators of a particle in the single-particle state with momentum modulus p:

$$\hat{H} = \sum \frac{p^2}{2m}\hat{a}_p^\dagger\hat{a}_p + \frac{U_0}{2V}\sum \hat{a}_{p+q}^\dagger\hat{a}_{p-q}\hat{a}_p^\dagger\hat{a}_p \tag{12}$$

where $U_0 = \frac{4\pi\hbar^2 a}{m}$ is the constant value of the two-body interaction in terms of the scattering length using the

Born approximation. The first summation is over p and the second one is over p_1 , p_2 and q.
We first consider the lowest approximation of the system energy and neglect all the terms where $p \neq 0$; we then consider all particles are in the lowest energy state $p = 0$. Applying the Bogoliugov approximation, we find the ground state energy of the system, $E_0 = \frac{1}{2}NV_0n$. With this result, we derive chemical potential of the dilute Bose gas, $\mu = mc^2$, and find the relation $c = \sqrt{U_on/m}$. The non-zero velocity of sound raises the possibility that phonons might play an important role in determining the low-temperature behaviour of the system.

We now carry out a higher-order approximation considering there are particles in states with $p \neq 0$. As this number is small, the fraction of particles in the state $p = 0$ is very close to one. Terms containing only one particle operator with $p \neq 0$ do not enter the Hamiltonian due to momentum conservation. By retaining all the quadratic terms in the particle operators $p \neq 0$ we obtain this expression for the Hamiltonian:

$$\begin{aligned}\hat{H} =& \frac{U_0}{2V}\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_0 + \sum_p \frac{p^2}{2m}\hat{a}_p^\dagger\hat{a}_p \\ &+ \frac{U_0}{2V}\sum_{p\neq 0}\left(4\hat{a}_0^\dagger\hat{a}_p^\dagger\hat{a}_0\hat{a}_p + \hat{a}_p^\dagger\hat{a}_{-p}^\dagger\hat{a}_0\hat{a}_0 + \hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_p\hat{a}_{-p}\right)\end{aligned} \tag{13}$$

To evaluate the energy levels of the system, we apply the Bogoliugov prescription and diagonalize the Hamiltonian with a linear transformation of operators $\hat{a}_p$ and $\hat{a}_p^\dagger$ in terms of independent quasi-particles creation operators $\hat{b}_p$ and $\hat{b}_p^\dagger$, to obtain:

$$\hat{H} = E_0 + \sum_{p\neq 0}\varepsilon(p)\hat{b}_p^\dagger\hat{b}_p, \tag{14}$$

with $\epsilon(p) = \sqrt{(cp)^2 + (p^2/2m)^2}$. This result show that the original system of interacting particles can be described in terms of a Hamiltonian of independent quasi-particles of energy $\epsilon(p)$ whose annihilation and creation operators of momentum p are given by $\hat{b}_p$ and $\hat{b}_p^\dagger$, these excitations correspond to phonons.

IV. LINEAR RESPONSE THEORY

Linear response theory is a powerful tool with which to explore the dynamic behaviour of interacting many-body systems at zero and finite temperatures used to describe how a system in equilibrium responds to external perturbations that are small enough for them to be treated as linear deviations from equilibrium. Consider the q component of the Fourier transform of the density operator $n(\vec{r}) = \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i)$.

$$\rho_q = \int d\vec{r}e^{-i\vec{q}\cdot\vec{r}}n(\vec{r}) = \sum_{i=1}^N e^{-i\vec{q}\cdot\vec{r}_i} \tag{15}$$

We can write the static structure factor of the system in terms of ρ_q.

$$S(q) = \frac{1}{N}(\langle\rho_q\rho_{-q}\rangle - |\langle\rho_q\rangle|^2) \tag{16}$$

We now use the method of sum rules, which is a useful tool in linear response to evaluate the moments of the dynamic structure factor:

$$m_v(F) = \hbar^{v+1}\int_{-\infty}^{+\infty} dww^v S(q,w) \tag{17}$$

where F is the external field applied on the system, v is the order of the moment and w represents the frequency of the perturbation. Using the linear response formalism, several useful inequalities can be derived. At $T = 0\,\mathrm{K}$, the dynamic structure factor vanishes for $w < 0$, leading to upper bounds for the energy $\hbar w$ of the lowest state $\hbar w \leq m_{p+1}/m_p$. Using the results of m_0 and m_1, we find [2]:

$$\epsilon_F(q) = \frac{m_1(q)}{m_0(q} = \frac{\hbar^2q^2}{2mS(q)} \tag{18}$$

To obtain the relation between the static structure factor and the excitation energy for the specific case of a weakly interacting Bose gas with $T << T_c$, we make use of the density matrix in the formalism of second quantization, $\rho_q = \sum_p a_{p-hq}^\dagger a_p$ and of the Bogoliugov approximation. Writing the density operator in terms of the creation and annihilation operators of quasiparticles using the Bogoliugov transformation, we obtain the expression [2]:

$$S(q) = \frac{\hbar^2q^2}{2m\epsilon(q)}\coth\frac{\epsilon(q)}{2k_BT} \tag{19}$$

which at the low temperatures we are working with simplifies to equation (18). This relation between the excitation energy and the static structure factor provides a qualitative explanation of the roton minimum exhibited by the energy spectrum in Fig. 3.

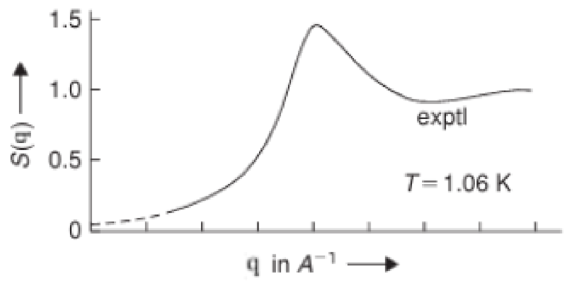

FIG. 4: Structure factor of liquid helium derived by Henshay(1960) [2] from experimental data on neutron diffraction.

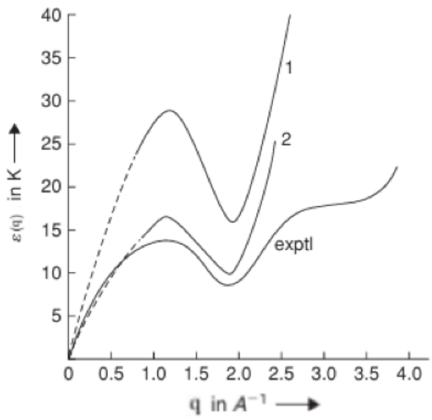

FIG. 5: The energy spectrum of the elementary excitations in liquid ^{4}He. Curve 1 shows the energy-momentum relationship based on equation (18) curve 2 is based on an improved formula by "Feynman and Cohen (1956) [5]". For comparison, the experimental results are also included.

Considering $S(q)$ shown in Fig.4, we see that its maximum results in the minimum of the energy spectrum, thus providing a consistent theoretical foundation for the manifestation for Landau's rotons; this is explicitly shown in Fig. 5.

V. THE CRITICAL VELOCITY FOR SUPERFLUIDITY

We end by considering a mass M in motion within the liquid in the superfluid phase. Its kinetic energy and momentum are $E = \frac{1}{2}Mv$ and $P = Mv$. A change in these quantities can be expressed as $\delta E = |\mathbf{v} \cdot \delta\mathbf{P}|$. Now we suppose that these changes result from the creation of an excitation $\epsilon(p)$ in the fluid. By conservation:

$$\delta E = -\epsilon \quad \text{and} \quad \delta\mathbf{P} = -\mathbf{p} \tag{20}$$

This implies $\epsilon = |\mathbf{v}\cdot\mathbf{p}| \leq vp$. An excitation cannot be created in the fluid unless its drift velocity is at least equal to (ϵ/p). We therefore find a condition for maintaining superfluidity:

$$v < v_c = \left(\frac{\epsilon}{p}\right)_{\text{min}} \tag{21}$$

The critical velocity v_c of the superfluid sets an upper limit for the maximum velocity at which a liquid in the superfluid state can flow. Observed values of v_c range between 0.1 cm/s and 70 cm/s. First of all, note that if the excitations followed the ideal gas $\epsilon(p)$ relation, v_c would be zero, making superfluidity impossible in the ideal case and highlighting the crucial role of interatomic interactions in producing a non-ideal excitation spectrum to enable superfluidity. While an ideal Bose gas can undergo Bose-Einstein condensation, it cannot exhibit superfluidity. For phonons, $v_c = c \approx 2.4\times10^4$ cm/s, and for rotons, $v_c \approx 6.3 \times 10^3$ cm/s, which are too high in comparison with the experimentally observed values. This indicates there must be another type type of collective excitations to break superfluid helium. This is indeed true. These excitations are quantized vortex rings, which are beyond the scope of this work.

VI. CONCLUSION

This TFG has conducted a study on various aspects related to superfluidity and its connection with Bose-Einstein condensation. Significant similarities between the ^{4}He superfluid transition phase and the condensation of ideal Bose gas in the lower energy state have been exposed. Phonon and roton have been predicted trough the study of superfluid ^{4}He elementary excitations.Using the formalism of second quantization, the condensate wave function has been determined, and the Bose-Einstein condensate excitations corresponding to phonons have been identified. Roton excitations have been successfully described by establishing the connection between the static structure factor and the excitation energy. Finally, through the study of the critical velocity of the superfluid, the existence of other excitations corresponding to quantized vortices has been revealed.

Acknowledgments

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Aspectes quàntics de la superfluidesa

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Resum: En aquest TFG s'ha estudiat la relació entre el fenomen de la superfluidesa i el condensat de Bose-Einstein, fent especial èmfasi en les excitacions del superfluid. S'estudia la mecànica estadística d'un gas ideal de bosons i s'obtenen resultats de capacitat calorífica i temperatura de transició de fase molt similars als experimentals de ^{4}He. S'estudien les excitacions del superfluid, predint-ne dues: els coneguts fonons i una altra anomenada rotons de Landau. Emprant mecànica quàntica, concretament el formalisme de segona quantització, es troba la funció d'ona del condensat i s'estudia l'energia del sistema, trobant així les excitacions corresponents als fonons. Es desenvolupa la teoria de resposta lineal aplicada a un gas poc interactuant i es troben les segones excitacions, els rotons. Finalment, es discuteix breument la velocitat crítica del superfluid i es conclou que hi ha d'haver un altre tipus d'excitació diferent, corresponent als anells de vòrtex.

Objectius de Desenvolupament Sostenible (ODSs o SDGs)

1. Fi de la es desigualtats		10. Reducció de les desigualtats	
2. Fam zero		11. Ciutats i comunitats sostenibles	
3. Salut i benestar		12. Consum i producció responsables	
4. Educació de qualitat		13. Acció climàtica	
5. Igualtat de gènere		14. Vida submarina	
6. Aigua neta i sanejament		15. Vida terrestre	
7. Energia neta i sostenible		16. Pau, justícia i institucions sòlides	
8. Treball digne i creixement econòmic		17. Aliança pels objectius	
9. Indústria, innovació, infraestructures			

VII. PARAULES CLAU

Heli , Superfluid , Funció d'ona, Hamiltonià, Fonó , Rotó