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Bose-Einstein Condensate and Superfluidity

M. Apostol
Department of Theoretical Physics, Institute of Atomic Physics,
Magurele-Bucharest Mg-6, POBox Mg-35, Romania
email: apoma@theory.nipne.ro

Abstract

The basic elements of the theory of the superfluidity are reviewed. The quantal hydrodynamics is discussed, and the quantal nature of the vortices is emphasized. It is stressed the essential role played by the cristalinely-ordered superfluid ground state, and the vortex and roton spectrum of a superfluid is derived. It is shown that quanta of vorticity it is also the quanta of viscosity, and the turbulence originates in quantal vortices. The vortex and roton spectrum is also derived by using a typical hard-core atomic potential, or a screened Coulomb potential with an oscillating tail. The condensate wavefunction is introduced allowing for the sound waves, vortices and rotons, and the quanta of these elementary excitations are thereby derived once more.

The 2001 Nobel Prize in Physics has been awarded for the "Bose-Einstein condensation in dilute gases of alkali atoms".[1]

In these experiments atomic beams of ^{87}Rb or ^{23}Na, which have an integral spin, and therefore we call them bosons, are slowed down by photons in laser beams, taking advantage of the frontal Doppler shift (for such techniques another Nobel Prize in Physics has been awarded in 1997). Optical and magnetic fields provide then magneto-optical traps for such cold atoms, while another laser beam or a rotating magnetic field polarize the atomic spins in the traps. Dilute alkali gases of several thousands of atoms in a space region of cca $1\mu m$ a scale length are thus obtained at a very low temperature of tens of $nK = 10^{-9}K$. In fact, such a temperature is sufficiently low for the average inter-atomic separation (several hundred of Å) to make these atomic ensembles very dilute quantal liquids of bosons undergoing Bose-Einstein condensation and superfluidity. Indeed, light scattering pictures the small, condensed liquid drop, spliting such a drop and thereafter bringing together the two fragments gives interference, as for a coherent atomic state, and many vortices are also observed in these superfluid droplets. All these are signatures of a Bose-Einstein condensation and superfluidity.

All this may be interesting laboratory techniques, experimental methods and procedures. However, they are not relevant for science. Bose-Einstein condensation and supefluidity are well-established and well-known, and He^4 superfluidity is known since 1911.[2]

If we are to consider an elementary particle and still care about its internal structure, then its internal coordinates vanish, its internal momenta go to infinite, so that, beside the internal energy, we may have, at most, a finite internal angular momentum, as an internal prime integral. This is $\hbar s$, where $\hbar$ is Planck's constant and s is called the spin of the particle. A spinning electron was suggested originally in connection with the Zeeman effect,[3] especially that a magnetic momentum is often associated with spinning particles (through the gyromagnetic factor), and assigned a quantal number of one half.[4] Indeed, as an angular momentum, its projection along one axis has $2s+1$ states, and $2s$ must be an integer; therefore, spin s may be an integer or half an integer. $2s+1$ states are described by a symmetric tensor of rank $2s$ whose labels take two values; this is called a spinor; it rotates under a rotation about one axis. It is worth noting that spin vanishes in the quasiclassical description. Particles with an integral spin are described by Klein-Gordon-type equations; the energy in this case is a quadratic form in particle fields plus a quadratic form in hole fields; it is positive defined providing the fields commute; if the fields commute the wavefunctions of identical particles are symmetric under particle permutations; if the wavefunctions are symmetric the occupation number of one-particle states may take any positive, integral value; consequently, particles of integral spins obey the Bose-Einstein statistics and are called bosons. Particles with a half-integral spin are described by Dirac-type equations; the energy in this case is a quadratic form in particle fields minus a quadratic form in hole fields; it is positive defined providing the fields anticommute; the wavefunctions of identical particles are then antisymmetric under particle permutations, and the occupation number of one-particle states may only take two values, zero and one. Consequently, such particles obey the Fermi statistics and are called fermions. This is the spin-statistics theorem.[5]

The constituents of a composite particle have both a total orbital momentum $\mathbf{L}$ and a total spin $\mathbf{S}$. The particle is invariant under rotations, so that its total angular momentum $\mathbf{J}=\mathbf{L}+\mathbf{S}$ is conserved; consequently, it is described by a symmetric spinor of rank $2J$, which have $2J+1$ components; therefore, $\mathbf{J}$ is its spin. The hamiltonian of the particle may contain additional terms like $\sim \mathbf{J}^2$, and the ground state corresponds to the lowest value $|L-S|$ of J, or to the highest $|L+S|$, depending on the sign of such terms (as the energy has a lower bound, the internal structure of composite particles being non-relativist, with relativist corrections; such an additional term comes usually from the spin-orbit interaction). The constituents of composite particles are frequently identical particles, like electrons in atoms, or nucleons in atomic nuclei. The energy levels of identical particles are labelled by the irreducible representations of the permutations group. For identical particles with spin one half these representations correspond to a well-determined total spin $\mathbf{S}$, and the dependence of the energy levels of two identical fermions of spin one half on their spin is the exchange interaction. The interacting particles building up a composite particle move in a self-consistent field, so that one-particle states are appropriate. The one-particle levels group themselves in energy shells, and the total spin and total orbital momentum in each shell is such as to minimize the energy, for the ground state of the composite particles. Consequently, for electrons, a shell has the highest possible spin and the highest possible orbital momentum (which is known as Hund's rule[6]), the corresponding symmetry of the wavefunction under permutations ensuring thereby as lowest an energy as possible, for the ground state. Closed shells have vanishing $\mathbf{L}$ and $\mathbf{S}$, while open shells have $J=|L-S|$ if they are less than half filled, and $J=L+S$ if they are more than half filled, according to the spin-orbit interaction. This way, having determined the energy shells, one may know the spin, the orbital momentum and the total angular momentum. For instance, $^{87}_{37}$Rb has a $...3d^{10}4s^24p^65s^1$ succession of shells, labelled by the principal quantal number n, orbital quantal number l $(0,1,2...$ correspond to $s,p,d...)$, the superscript indicating the total number of electrons in the shell; consequently, the total spin of the electrons is $S=1/2$, the total orbital momentum is $L=0\,(S)$ and the total angular momentum is $J=|L-S|=1/2$, as given by the open upper shell (the ground state is therefore labelled by the electronic term $^2S_{1/2}$, *i.e.* $^{2S+1}(L)_J$). Similarly, $^{23}_{11}$Na has a $^2S_{1/2}$ ground state, with a $...2p^63s^1$ upper shell. For nucleons the difference is made by the fact that the nuclear forces depend on spin, so that the self-consistent field gives rise to a stronger "spin-orbit" interaction, which, accordingly, classifies the energy bands by the angular momentum $\mathbf{j}$ of the nucleon. The nucleon states are labelled by nl_j, where the principal quantal number $n = 1, 2, ...$ and the orbital quantal number $l = j \pm 1/2$ is well-defined, as the nucleon states have a well-defined parity. The nucleon shells are [7] $(1s_{1/2})$, $(1p_{3/2}, 1p_{1/2})$, $(1d_{5/2}, 1d_{3/2,} 2s_{1/2}, 1f_{7/2})$, $(2p_{3/2}, 1f_{5/2}, 2p_{1/2}, 1g_{9/2})$, etc. The band filling is dictated by the nuclear pairing which couples nucleon pairs at a vanishing angular momentum, so that the even-even nuclei *(i.e.* an even number Z of protons and an even number $A - Z$ of neutrons) have a vanishing total angular momentum $J = 0$, odd-even nuclei have a total angular momentum $J = j$ of the upper unpaired nucleon, and the odd-odd nuclei have a total angular momentum $J = 2j$; indeed, in the later case the isotopic spin ($T = 0$) corresponds to an antisymmetric wavefunction, and the rest of the wavefunction (spin and coordinate parts) must be symmetric. For instance, the 37 protons of $^{87}_{37}$Rb are arranged in a closed shell of 28 and an open shell $...2p_{3/2}\, 1f_{5/2}\, 2p_{1/2}\, (1g_{9/2})$ with one unpaired proton on $1f_{5/2}$; consequently, the nuclear spin of $^{87}_{37}$Rb is $I = 5/2$. Similarly, $^{23}_{11}$Na should have a nuclear spin $I = 5/2$; however, it is an exception and has $I = 3/2$ a nuclear spin. The spin of the atom is therefore $\mathbf{F} = \mathbf{J} + \mathbf{I}$, which is conserved, and the hamiltonian contains the electron-nucleus hyperfine interaction $\sim \mathbf{F}^2$; this interaction always tends to anti-allign the spins, by the effect of the magnetic field, so that the atomic spin in the ground-state is $F = |J + I|$; for $^{87}_{37}$Rb and $^{23}_{11}$Na the atomic spins are therefore $F = 2$ and $F = 1$, respectively.

The statistical distibution for identical particles with integral spin has been introduced by Bose.[8] Einstein noticed that at low temperatures such particles occupy the lowest energy level, such as to accommodate the macroscopic number of particles.[9] This is the Bose-Einstein condensation. Its connection with the superfluidity of He^4 has been suggested by London.[10] However, the Bose-Einstein condensation is a third-order phase transition, while the supefluidity is a second-order one. The superfluid transition is described by the Ginsburg-Landau theory,[11] while the superfluidity by Landau.[12] It is the excitation spectrum of the condensate which is relevant for superfluid properties; it consists of sound-like phonons for long wavelengths and vortices and rotons for shorter wavelengths.[12] The sound-like phonons were derived as long-wavelengths elementary excitations of an interacting Bose-Einstein condensate,[13] while vortices and rotons are suggested, in a certain sense, by Gross-Pitaevskii equation.[14] The interaction of the Bose quantal liquid is repulsive, and the Bose-Einstein condensation is preserved for an interacting liquid of bosons.[15]

The attractive part of the interaction of some kinds of atoms may not be strong enough to solidify them under normal pressure even at vanishing temperatures, especially for lighter atoms; consequently they form quantal liquids; the typical examples are He^4 below ~ 2.17K and He^3 below ~ 3.2K; the former is a Bose quantal liquid, while the latter is a Fermi quantal liquid. While the atoms in a quantal liquid move quasi-freely over most part of their paths, they may experience strong collisions with each other, due to the repulsive part of the interaction. Apart from such collisions the atoms are otherwise weakly interacting, which explains why the Bose-Einstein condensation is possible in an interacting quantal liquid of bosons, and why the interaction effects are perturbation-like in a quantal liquid of fermions. However, the effects of the interaction are quite distinct for bosons and for fermions, as a consequence of their distinct statistics.

Let such a quantal liquid of bosons be in its ground state, at vanishing temperature, where all the atoms are on the zero energy levels (actually, on the same one-particle state with zero energy). Any interaction takes such a quantal liquid from its ground state to its excited states; the later are characterized by an energy, and, sometimes, by a momentum; their quanta are called elementary excitations.[12] Small, long-wavelengths, longitudinal disturbances of the liquid density may propagate above the ground state, governed by the repulsive interaction; they are quanta of sound, and are the basic excitations of the Bose-Einstein condensate; they have a momentum. For a given momentum there are no other excitations below the sound quanta in the Bose-Einstein condensate, and this is the basic point explaining the superfluidity. Indeed, a slightly excited atom would soon fall down in the condensate, as a consequence of the Bose-Einstein statistics, in contrast to the Fermi statistics where the fermions may assume individually excited states (or in contrast also with a classical liquid); in this latter case the excitations are quasiparticles, and they may have vanishing energies. Therefore, an excited Bose-Einstein condensate may only take an energy and a momentum corresponding to the dispersion relation of the sound quanta, *i.e.* internal motion with velocities smaller than the sound velocity are allowed without viscosity within the liquid; this is the superfluid phenomenon. Indeed, a mass M of a fluid moving with v velocity has an energy $Mv^2/2$, and a small change δv in the velocity means an energy change $\varepsilon = Mv\delta v = vp$, where p is the momentum; to excite a sound quanta ε must be as large as the sound quanta of energy up at least, where u is the sound velocity; *i.e.* $vp > up$; for $v < u$ the motion proceeds without loss, *i.e.* without viscosity, *i.e.* the liquid is superfluid. It is easy to see that heat also is not propagated into a superfluid. However, for velocities v finitely smaller than sound velocity u the superfluidity is nevertheless destroyed, which suggests another kind of elementary excitations, lying close to a finite momentum and having a quadratic dispersion around an energy gap; such excitations were called rotons and the energy gap assigned to localized vortices.[12]

Indeed, the average inter-atomic separation a in a Bose liquid plays a relevant role. Since the bosons may assume identical states, the effect of their interaction is local, in contrast with fermions, where the interaction acts globally, in accordance with their assuming individual states only. A localized effect of the interaction may lead to localized excitations for bosons, over distances of the order of a, obviously corresponding to a momentum of the order of $1/a$, and having a finite energy gap; the energy gap is of the order of $\hbar^2/ma^2$, where m is the atomic mass (and $\hbar$ denotes Planck's constant). Such excitations lie below the sound quanta in energy at that $1/a$ momentum, for obvious reasons, too (as for a liquid); such excitations are called vortices, for reasons to be seen shortly. Moreover, the excitations of such vortices, to say so, are called rotons and, obviously, they are particle-like excitations, *i.e.* their spectrum is $p^2/2\mu$ with respect to the vortices, where μ is an effective mass. Everything happens as if an atom is caught in a cage made of the surrounding atoms, where it moves around, together with its surounding. It is also worth noting that the interaction is "removed" in such a picture, as if its effects were solved out.

The local effects of the interaction being important for a Bose liquid, it is then appropriate to view it as a quantal fluid, described by local quantities. Indeed, Landau [12] quantized the motion of a fluid starting with a particle (mass) density $\rho = \sum m\delta(\mathbf{r}-\mathbf{R})$ and a (mass) flow of particles $\mathbf{j} = (1/2)[\sum \mathbf{p}\delta(\mathbf{r}-\mathbf{R}) + \delta(\mathbf{r}-\mathbf{R})\mathbf{p}]$, where the particles are placed at $\mathbf{R}$. Obviously, this is a $\psi(\mathbf{r})$ field theory, the particle density being $\psi^+(\mathbf{r})\psi(\mathbf{r})$ (mass density being $\rho(\mathbf{r}) = m\psi^+(\mathbf{r})\psi(\mathbf{r})$) and the mass flow being $\mathbf{j}(\mathbf{r}) = (1/2)[\psi^+(\mathbf{r})\cdot\mathbf{p}\psi(\mathbf{r}) - \mathbf{p}\psi^+(\mathbf{r})\cdot\psi(\mathbf{r})]$. A velocity field $\mathbf{v}(\mathbf{r}) = (1/2m)[\psi^+(\mathbf{r})\cdot\mathbf{p}\psi(\mathbf{r}) - \mathbf{p}\psi^+(\mathbf{r})\cdot\psi(\mathbf{r})]$ is also introduced,[16] and commutation relations

$$v_i(\mathbf{r})v_k(\mathbf{r}') - v_k(\mathbf{r}')v_i(\mathbf{r}) = -(i\hbar/2m)\delta(\mathbf{r}-\mathbf{r}')(curl\mathbf{v})_{ik} \tag{1}$$

are found, where i, k denote the components of the velocities and $(curl\mathbf{v})_{ik} = \partial v_k/\partial x_i - \partial v_i/\partial x_k$. These are the basic equations which led Landau to substantiate the idea of vortices and rotons; their main characteristics is their inhomogeneity in velocities, *i.e.* the *lhs* of (1) is of second-order in velocities while the *rhs* of (1) is of first order in velocities; and, of course, the non-vanishing commutator in (1).

Before analyzing equation (1) with respect to vortices and rotons it is worth making some remarks. First, such a quantal hydrodynamics, *i.e.* a local field theory, is generally valid for any quantal liquid ((1) including). However, it is superfluos to a great deal of extent for fermions, because the excited states therein are delocalized, and the *curl* of a velocity near the (large) Fermi velocity is vanishing, as the change in such a velocity proceeds by vanishing changes in momenta. This is why one prefers to work with global quantities in the second quantization for fermions, *i.e.* with integrating densities of the type above over the whole volume of the liquid. The two formalisms, by the way, *i.e.* the local quantal hydrodynamics on one side, and the global second-quantized field theory on the other, already contain in themselves the solution of the interaction problem for bosons and for fermions, respectively, which sounds remarkably. Secondly, it is worth noting that the field $\psi(\mathbf{r})$ is analyzed in plane waves, as usually, making the understanding of (1) much more available. Further on, it is worth stressing that the velocity $\mathbf{v}(\mathbf{r})$ introduced above is a field operator, *i.e.* an operator in the occupation number of plane waves. In particular, the average velocity $\mathbf{v} = (-i\hbar/2m)[\psi^*(\partial\psi/\partial\mathbf{r}) - (\partial\psi^*/\partial\mathbf{r})\psi]$, where $\psi \sim e^{i\Phi}$ is a wavefunction is $v = \hbar grad\Phi/m$, and its *curl* is always vanishing, of course (and *curl*$\mathbf{v}$ is off-diagonal). Also, the velocity as defined above can be written as

$$\mathbf{v}(\mathbf{r}) = (\hbar/2m)\sum(2\mathbf{k}+\mathbf{q})a^+_{\mathbf{k}}a_{\mathbf{k}+\mathbf{q}}e^{i\mathbf{qr}} \quad , \tag{2}$$

where $a^+_{\mathbf{k}}, a_{\mathbf{k}}$ are creation and destruction operators, respectively, of plane waves; now, one can see easily that a longitudinal wave has a vanishing *curl* of velocity, so that the sound waves are not affected by (1), and the velocity of a quasiparticle excitation close to the Fermi surface has a vanishing *curl* too. Moreover, the *curl* of velocities is the highest for both $\mathbf{k}$ and $\mathbf{q}$ close to the highest relevant wavevectors, *i.e.* wavevectors of the order of $1/a$; it follows that (1) involves motion localized over the average inter-atomic separation a and interaction processes that exchange $\sim \hbar/a$ momenta; and such a movement is relevant for bosons, and it may be called a vortex as the *curl* of its velocity is non-vanishing. It is also worth noting that such atomic movements are spatially disentangled from each other, as (1) is effective only at the same location. It follows also that any motion in the superfluid state, *i.e.* a motion with a velocity $\mathbf{v}$ low enough as not to excite vortices is potential, *i.e.* irrotational, *i.e.* $curl\mathbf{v} = 0$. Indeed, if $curl\mathbf{v}$ is zero everywhere it commutes with everything, with the hamiltonian too, and is conserved.

Indeed, the hamiltonian of an interacting ensemble of particles reads

$$H = \sum \mathbf{p}^2/2m + \frac{1}{2}\sum v(\mathbf{R}-\mathbf{R}') \tag{3}$$

(spin neglected), or

$$H = \sum(\mathbf{p}^2/2m)a^+_{\mathbf{p}}a_{\mathbf{p}} + (1/2V)\sum v(\mathbf{q})a_{+\mathbf{p}_1}a_{+\mathbf{p}_2}a_{\mathbf{p}_2-\hbar\mathbf{q}}a_{\mathbf{p}_1+\hbar\mathbf{q}} \quad , \tag{4}$$

where $v(\mathbf{q}) = \int d\mathbf{r}\cdot v(\mathbf{r})e^{i\mathbf{qr}}$ and V is the volume of the ensemble; and one can easily recognize the density $n(\mathbf{r})$ in the interacting term in (3) and (4), and a displacement field $\mathbf{u}(\mathbf{r})$ produces a change $\delta n = -ndiv\mathbf{u}$ in density; for bosons one gets straightforwardly the frequency $\omega = [nv(\mathbf{q}=0)/m]^{1/2}q$ of longitudinal sound waves; similarly, one may obtain sound for fermions too (where the contribution of kinetic energy must be included), but it is unstable against the quasiparticle excitations.[17] Further on, $curl\mathbf{v}$ does not commute with the kinetic hamiltonian (though it commutes with density; and with itself too!), so that it has no defined values for the elementary excitations, except for those which are longitudinal (when it vanishes); therefore, a vortex (with defined energy) has no well-defined *curl*, and, conversely, a well-defined *curl* has no well-defined energy. Moreover, $curl\mathbf{v} \neq 0$ requires a non-vanishing velocity in order to satisfy the inhomogeneous (1), so that such a vortex must have a finite energy, *i.e.* a gap in the excitations energy. (In addition, it is worth noting that the quantal hydrodynamics obeys the continuity equation and Euler's equation of motion for fluids). Obviously, a local non-vanishing velocity may only arise from interaction processes exchanging momenta of the order of $\hbar/a$. For such interaction processes one obtains an average velocity $v \sim (\hbar/m)(\sin r/a)/r$ from (2), whose *curl* is $curl\mathbf{v} \sim (\hbar/ma)(\cos r/a)/r$ (having no definite orientation $\mathbf{v}$ does not come from a *grad*). The integral $\int d\mathbf{s} \cdot curl\mathbf{v}$ over any surface around the point is then the circulation $\oint d\mathbf{l} \cdot \mathbf{v}$ of the velocity around that point, and equals $\sim \hbar/m$.[18] It is called vorticity, and its quanta is h/m ($\hbar = h/2\pi$;) it is the same as quanta of viscosity,[19] for obvious reasons; indeed, the origin of viscosity is quantal (it is worth noting in this connection that the quantal uncertainty in the fermion quasiparticle energy originates in a vortex too), and the classical turbulence is made of quantal vortices. In particular, one can notice that $curl\mathbf{v} \sim \mathbf{p} \times \mathbf{v}$, which is a purely quantal quantity.

The ground-state of a liquid consisting of identical interacting bosons is a crystalinely-ordered state, characterized by a set of three reciprocal vectors $\mathbf{G}$, the atoms being placed at $\mathbf{R}_i$. Atoms, however, may oscillate within their atomic cages, with very low energies, and $\hbar\mathbf{g}$ momenta, where $\mathbf{g}$ is a multiple $n\mathbf{G}$ of $\mathbf{G}$. The average of the structure factor $\sum e^{i\mathbf{q}\mathbf{R_i}}$ gives $\mathbf{g}$-peaks decreasing like $1/q^3$, as for a genuine liquid with short-range order. Delocalized states, like an atom travelling with momentum $\hbar\mathbf{k}$, are therefore identical with "umklapp" scaterred states, in particular an atom travelling with a momentum $\hbar(\mathbf{k}+\mathbf{g})$; therefore, $a_{\mathbf{k}+\mathbf{g}}$ can be replaced by $a_{\mathbf{k}}$. Only $\mathbf{G}$-scattering processes may be kept in collisions, in view of the "short-range" character of the interaction, so that the velocity (2) becomes

$$\mathbf{v}(\mathbf{r}) = (\hbar/m\mathbf{k})a^+_{\mathbf{k}}a_{\mathbf{k}}\sum e^{i\mathbf{G}\mathbf{r}} \quad , \tag{5}$$

for one particle, where the summation extends over $\mathbf{G}$'s; correspondingly, its *curl* is

$$curl\mathbf{v} = i(\hbar/m)\sum(\mathbf{k}\times\mathbf{G})a^+_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{G}\mathbf{r}} \quad , \tag{6}$$

and one can see they are diagonal now in the particle occupancy; but, of course, they do not commute anymore with the hamiltonian now, in particular with the $\mathbf{G}$-interaction processes in (4). For a vortex, the particle momentum is $\mathbf{g}$ in principle (actually of the order of $\mathbf{G}$ in fact), and its energy (minimal) is of the order of $\Delta = \hbar^2/ma^2$ (for $He^4 \sim 9$K from neutron scattering,[20] while $a \sim 3.7$Å). A particle may escape a vortex after at least one planar loop involving 4 $\mathbf{G}$-collisions; its energy is then $\hbar^2(k^2+4G^2)/2m$, and for $k \sim G$, it involves an effective mass $\mu \sim m/5 = 0.2m$ (the experimental value from neutron scattering is $0.16m$ for He^4). In addition, it is worth noting the position of the vortex gap at $G \sim 1/a$, actually at $2\pi/a = 1.7$Å^{-1}; the experimental location is 1.9Å^{-1}; and the roton energy $\mathbf{p}^2/2\mu$ which is quadratic in momenta. From (5) and (6) one can see again that the vorticity is $\sim nh/m$, *i.e.* is quantized in h/m-quanta, and *curl* is represented as $\hbar/m(\mathbf{g}\times\mathbf{G})$, where $\mathbf{k} \sim \mathbf{g}\,(\sim \mathbf{G})$.

The ground-state of (4) is a condensate with all $\mathbf{p} = 0$; its elementary excitations consist of pairs of interacting particles; following Ref.13 one gets straightforwardly

$$\begin{aligned} H = \tfrac{1}{2}Nnv(0) + \tfrac{1}{2}n^2\sum\tfrac{v^2(\mathbf{p})}{p^2/m} + \sum(\mathbf{p}^2/2m)a^+_{\mathbf{p}}a_{\mathbf{p}} + \\ +\tfrac{1}{2}n\sum v(\mathbf{p})[a^+_{\mathbf{p}}a^+_{-\mathbf{p}} + a_{-\mathbf{p}}a_{\mathbf{p}} + 2a^+_{\mathbf{p}}a_{\mathbf{p}}] \end{aligned} \tag{7}$$

for the hamiltonian of these excitations; it is worth noting that the excitations contributions are consistently included in (7) up to the second order of the perturbation theory, and the ground-state energy is accordingly renormalized by the second term in the *rhs* of (7). The diagonalization of the hamiltonian above is straightforward, and the excitation spectrum is given by

$$\varepsilon(\mathbf{p}) = [nv(\mathbf{p})p^2/m + (p^2/2m)^2]^{1/2} \quad , \tag{8}$$

while the ground-state energy reads

$$E_0 = \frac{1}{2}Nmu^2 + \frac{1}{2}n^2\sum\frac{v^2(\mathbf{p})}{p^2/m} + \frac{1}{2}\sum\{\varepsilon(\mathbf{p}) - [p^2/2m + nv(\mathbf{p})]\} \quad , \tag{9}$$

where $u = \sqrt{nv(0)/m}$ is the sound velocity (~ 240m/s); carying out the integration in (9) one gets $E_0 = (1/2)Nmu^2[1 + \alpha(mu)^3/2\pi^2\hbar^3 n]$, where α is slightly smaller than the usual value $\alpha = 2.3$ corresponding to a δ-type interaction ($v(\mathbf{p}) = v(0)$). For typical hard-core atomic potentials the experimental spectrum of excitations is obtained from (8); similarly, it is given by screened Coulomb potentials with oscillatory tails. The excitations spectrum (8) can also be put in another form; indeed, denoting $\varepsilon_0 = p^2/2m$ one gets from (8) $\varepsilon = \varepsilon_0(1+nv(\mathbf{p})/\varepsilon_0)$ for large p; on the other hand the pair distribution function is given by $S(\mathbf{q}) = (1/N)\sum e^{i\mathbf{q}(\mathbf{R_i}-\mathbf{R_j})} = \sum' e^{i\mathbf{q}\mathbf{R_i}}$ (where N is the number of atoms and prime means summation over neighbours), and the potential can be written as $\overline{v} = \sum v(\mathbf{r}-\mathbf{R_i}) \sim nv(\mathbf{q})S(\mathbf{q})$ for $q \sim 1/a$; therefore, $\varepsilon = \varepsilon_0(1+\overline{v}/S(\mathbf{q})\varepsilon_0)$; in addition, the energy of the excitation can also be written approximately as $S\varepsilon_0 + \overline{v} = \varepsilon_0$ for the movement of an atom around its position $\mathbf{R_i}$, hence $\varepsilon = \varepsilon_0/S(\mathbf{q}) = \hbar^2 q^2/2mS(\mathbf{q})$, as suggested in Ref. 15.

The excitations of the superfluid form its normal component, while the remaining part is the superfluid component; they have distinct densities, and a two-fluid picture holds for superfluidity, as suggested earlier.[21] Sound, vortices and rotons do scatter on each other in the normal part of the superfluid, and the corresponding cross-section can be estimated.[22] The superfluid flows frictionlessly through capillaries and narrow slits, in a rotating vessel the superfluid does not rotate, has no inertia momentum (it is incapable of rotational flow), exerts no pressure on an immersed body (Euler's paradox); since the normal part and the superfluid part are in equilibrium there is no entropy transfer between them, and, of course, no friction and no viscosity in the relative motion of the two fluids one against the other. The superfluid flows like an "ordered" fluid, without changing the entropy, and does not carry heat (and the superfluid motion is thermodynamically reversible); and, of course, it is so at zero temperature, practically; flowing out of vessels and carying no heat the superfluid leaves behind the heat which boils the remaining fluid (this is the thermomechanical effect). The heat is transported by the normal fluid, which flows to the cold temperatures, while the superfluid flows in compensation to the warmer temperatures; this out-of phase mutual flow of the two fluids may proceed by temperature waves, which are called the second sound, and whose velocity is $u/\sqrt{3}$ at vanishing temperature, in contrast to the usual u-sound which is called the first sound too. Indeed, the interaction of the phonons with atoms gives Boltzmann's equation $\partial f/\partial t + (uq_i/q)\partial f/\partial x_i = I$ for their distribution function f, where I is the collision integral; introducing momentum $P_i = \int q_i f$ and energy $E = u\int(q_i^2/q)f$ one gets $\partial P_i/\partial t + (1/3)\partial E/\partial x_i = 0$ as well as $\partial E/\partial t + u^2\partial P_i/\partial x_i = 0$ (collisions do conserve the momentum and energy), hence $\partial^2 E/\partial t^2 - (u^2/3)\partial^2 E/\partial x_i^2 = 0$ and the second sound velocity $u/\sqrt{3}$.

It is now worth turning back to vortices. One may notice for the beginning that vortices given by (5) and (6) do not commute indeed with the hamiltonian (7). The wavefunction of a fluid moving with the velocity $\mathbf{v}$ has the form $\psi \sim \exp(im\mathbf{v}\sum\mathbf{R}/\hbar)$, and for a fluid rotating with the angular velocity ω the circulation of this velocity on a closed loop is of course $\oint \mathbf{dl}\cdot\mathbf{v} = (h/m) \times integer$ from the periodicity of the wavefunction, *i.e.* it is quantized by h/m, and its *curl* is 2ω; obviously, $v = \omega r = (L/m)/r$ in this case, and the vorticity is nothing but the quantization of the angular momentum L, and its *curl* is vanishing then. Such a motion is called a "vortex" too, but of course $\mathbf{v}\sum\mathbf{R} = 0$ in this case; it was suggested[23] that space is disconnected, and has a "hole", for instance at the centre, in which case ψ would go like $\psi \sim \exp(i\varphi(\mathbf{R})/\hbar)$; however $\mathbf{v} = (\hbar/m)grad\varphi$ would have no *curl* then, but, nevertheless, it is supposed further on that it may have a singularity at the "hole", where its *curl* might be non-vanishing, and Stokes' theorem would be used on the external loops only; in which case such a vortex might probably be better called a "circulating vortex", or an L-vortex, in contrast with a "*curl*, or an ω-, vortex". In any case it has nothing to do with the superfluid excitations called vortices. Nevertheless, such an irrotational motion does exist of course, with $v = \omega r = L/mr$, and the energy associated with one quanta of rotating velocity is the centrifugal energy $\int \pi r dr \cdot nm(\hbar/mr)^2 d$, *i.e.* $\pi n(\hbar^2/m)\ln(b/a)$ per unit depth d of the liquid; which is not compensated by the surface tension of a real hole; however, many such "linear holes", *i.e.* cylinders, do appear in a rotating superfluid, whose free surface is finely rigged with them, such as to minimize the energy and conserve the angular momentum, and they are related with the capacity of the superfluid of creating internal non-uniformities of a normal fluid, by exciting true vortices.

Let $\psi(\mathbf{r}, q)$ be the wavefunction of an ensemble of particles, for one particle at $\mathbf{r}$ and the rest with coordinates q. The one-particle density matrix $\rho(\mathbf{r} - \mathbf{r}') = \int dq\psi^*(\mathbf{r}, q)\psi(\mathbf{r}', q)$ has the Fourier transform $\int d\mathbf{R}\rho(\mathbf{R})e^{i\mathbf{kR}} = (1/V)\int dq\,|\psi(\mathbf{k}, q)|^2$, and $(1/V)\,|\psi(\mathbf{k}, q)|^2$ is the probability for one particle of being on the $\mathbf{k}$-state; for a condensed Bose liquid all the particles are deployed on the state $\mathbf{k} = 0$, so that $\rho(\mathbf{r})$ is finite at infinite; this is an off-diagonal long-range order.[24] What is more interesting is that the condensate has a field a_0, or, for a non-uniform condensate moving with some velocity, a $\psi(\mathbf{r}) = a(\mathbf{r})e^{i\phi(\mathbf{r})}$ field, where $a(\mathbf{r})$ is the amplitude and $\Phi(\mathbf{r})$ is a phase; this is a classical field (though for a quantal object), and is called the wavefunction of the condensate; the velocity is $\mathbf{v} = (\hbar/m)grad\Phi$ and is irrotational ($curl\mathbf{v} = 0$), as for a superfluid condensate. It is easy to see that $\psi(\mathbf{r})$ obeys

$$(-\frac{\hbar^2}{2m}\Delta - \mu)\psi(\mathbf{r}) + v(\mathbf{r} = 0)a^3\,|\psi(\mathbf{r})|^2\,\psi(\mathbf{r}) = 0 \qquad (10)$$

for a δ-potential, which minimizes the classical energy for an average number of particles (μ is the chemical potential); this is the Gross-Pitaevskii equation,[14] and describes non-uniformities of a moving condensate; in particular, it gives a depletion of the superfluid near a wall (and the surface tension of the superfluid), as well as cylindrical "circulating vortices" for a rotating supefluid ($v_\theta \sim 1/r$); in the latter case ψ goes like $\psi \sim e^{i\theta}$ and it is read $\psi \sim e^{iL\theta/\hbar}$, corresponding to an angular momentum $L = \hbar$; and the velocity reads $v_\theta = L/mr$; it has nothing to do with the true superfluid "*curl* vortices" (which, in particular, are associated with a hard-core potential). It is worth noting that the other two components of the angular momentum are vanishing as for a vanishing macroscopic rotation of the cylindrical vortex about the corresponding directions. Superfluid motion of non-uniform Bose condensates, as well as their long-wavelengths excitations, or macroscopic flows, superfluid hydrodynamics, including phase interference, Josephson-like oscillations of the flows, etc, are described by the Gross-Pitaevskii equation (10),[25] which amounts, for these reasons, to a mean-field theory; beyond this mean-field regime the picture is dominated by the atomic limit of the true *curl*-, quantal vortices.

Because the condensate does not conserve the number of particles (and its gauge symmetry $a_\mathbf{p} \rightarrow a_\mathbf{p}e^{i\varphi}$ is broken, as one can see, for instance, from (7)); and, in order to allow for the excitations in the condensate, it must be written as

$$\psi(\mathbf{r}) = \sqrt{n}(1 - \frac{1}{2}div\mathbf{u})e^{i\Phi} \quad , \qquad (11)$$

where $\mathbf{u}$ is the slowly varying long-wavelengths sound field, while Φ is associated with all the rest of possible movements, macroscopic motion included. Indeed, $|\psi(\mathbf{r})|^2 = n(1 - div\mathbf{u})$ is the change in density, while Φ-motion does not change the density; of course, including excitations the condensate wavefunction (11) has to be quantized; for the beginning it may be viewed as a quasiclassical description. In addition, the macroscopic motion may be left aside, and the phase Φ may be viewed as varying abruptly over atomic distances near a given position; the direction of its variation varies continuously, and this is the sense in which it describes a quasiclassical motion; otherwise, due to its localization and to the uncertainty in the direction of its variation, it corresponds to a quantal motion. The energy can easily be derived from (3) as

$$H = \int d\mathbf{r}\cdot\psi^+(\mathbf{p}^2/2m)\psi + \frac{1}{2}\int v(\mathbf{r}-\mathbf{r}')\psi^+(\mathbf{r})\psi^+(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) =$$

$$= \frac{\hbar^2 n}{2m}\int d\mathbf{r}\cdot|grad\Phi|^2 + \frac{1}{2}n^2\int v + \frac{1}{2}n^2\int v\cdot(div\mathbf{u})(\mathbf{div'u}) = \tag{12}$$

$$= \frac{\hbar^2 n}{2m}\int d\mathbf{r}\cdot|grad\Phi|^2 + \frac{1}{2}n^2 V\sum v(\mathbf{q}) + \frac{1}{2}n^2 V\sum v(\mathbf{q})q^2 u^*_{\mathbf{q}}u_{\mathbf{q}}\ .$$

With the kinetic term $\int d\mathbf{r}\cdot mn|\partial\mathbf{u}/\partial t|^2/2$ one gets the sound quanta $\omega = \sqrt{nv(0)/m}q$ for the $\mathbf{u}$-motion in (12). For the Φ-phase in (11) one may take $\Phi = gu$ according to the discussion above, where u is the displacement along a wavector $\mathbf{g}$ of the order of the reciprocal vector $\mathbf{G}$ (in which case the direction of the phase variation may also be quantized). The displacement u is developed in Fourier series as $u = \sum u_{\mathbf{g}}e^{i(\mathbf{g}+\mathbf{q})\mathbf{r}}$, where $\mathbf{q}$ is very small in comparison with $\mathbf{g}$ (so that $n\int d\mathbf{r} = 1$). The gradient of the phase can be represented as $grad\Phi \sim -\mathbf{g}u/a + g\cdot gradu$, since $gradg \sim -\mathbf{g}/a$, so that the velocity is $\mathbf{v} \sim (\hbar/m)(-\mathbf{g}u/a + g\cdot gradu)$, and its $curl\mathbf{v} \sim -i(\hbar/ma)\sum\mathbf{g}\times\mathbf{g}'u_{\mathbf{g}'}e^{i\mathbf{g}'\mathbf{r}}$ is non-vanishing. The corresponding energy as estimated from (12) is given by

$$\frac{\hbar^2}{2m}(g^2|u_{\mathbf{g}}|^2/a^2 + g^2|u_{\mathbf{g}}|^2/a^2 + g^2q^2|u_{\mathbf{g}}|^2) \simeq$$

$$\simeq \{\hbar^2(ag)^2/ma^2 + (ag)^2p^2/2m\}a^+_{\mathbf{g}}a_{\mathbf{g}}\ , \tag{13}$$

where $u_{\mathbf{g}} \sim aa_{\mathbf{g}}$; for $ag = \pi$ one obtains an energy $\Delta + p^2/2\mu$, where $\Delta = \pi^2\hbar^2/ma^2 \simeq 8\mathrm{K}$ and $\mu = m/\pi^2 \simeq 0.1m$ for He^4, which is the rotons spectrum. (It is worth noting that $\sum\mathbf{gq} = 0$ in (13)). However, $curl\mathbf{v}$ does not commute with (13); it may be viewed as a spin $\mathbf{S}$ of magnitude one, as corresponding to the vector $\mathbf{g}$, in which case the energy is represented as $(\mathbf{S}\mathbf{u}_{\mathbf{g}})^2$, but still $\mathbf{S}$ is not determined. Rotons and the superfluid vortices are purely quantal particles. In addition. phase is not determined, as for a determined number of atoms (one), and this is a phase diffusion.

However, it is energetically favourable for vortices turning about the same direction to get together, forming larger vortices (and antivortices) which are classical, and are "*curl* vortices"; however, they create discontinuities in the superfluid velocity, associated with the surface tension, and the free surface of a rotating superfluid is rippled with such layers of discontinuity.[26] The superfluid velocity goes like $1/r$ in such a rotating fluid, as for conserving the angular momentum (and like in Gross-Pitaevskii equation), and of course it is irrotational (and flow conserving, $div\mathbf{v} = 0$), and at least one true vortex there exists at the centre.

There is still another equivalent representation of the wavefunction (11). Indeed, the long wavelengths part can also be written as $\psi = \sqrt{n}e^{iu/a}$, and the density is given by $\psi^+(\mathbf{r} - i\mathbf{a}/2)\psi(\mathbf{r} + i\mathbf{a}/2) = n(1 - \mathbf{a}gradu/a) = n(1 - div\mathbf{a}u/a) = n(1 - div\mathbf{u})$; this form of the wavefunction shows up the condensate interference. A classical phase, *i.e.* a determined phase corresponds to an undetermined number of particles, and these are so indeed, as the atomic distances are uncertain. As regards the vortex part of the wavefunction (11) the phase Φ may be written as $(1/\hbar)\int p_r dr + (1/\hbar)\int p_\theta r d\theta + (1/\hbar)\int p_\varphi r\sin\theta d\varphi$ in spherical coordinates, which means

$$(1/\hbar)\int p_r dr + (1/\hbar)\int L_\varphi d\theta - (1/\hbar)\int L_\theta\sin\theta d\varphi\ , \tag{14}$$

where $\mathbf{L}$ is the angular momentum; in particular $L_\theta\sin\theta = L_z$, and $L_\varphi = rp_\theta$, $L_\theta = -rp_\varphi$. Therefore,

$$grad\Phi = \frac{1}{\hbar}(p_r,\ L_\varphi/r,\ -L_\theta/r) = \frac{m}{\hbar}(v_r,\ r\omega_\varphi,\ r\sin\theta\cdot\omega_z)\ , \tag{15}$$

where angular frequencies $\omega_{\varphi,z}$ are introduced as for a free angular motion. One can see that $curl\mathbf{v} = (2\cos\theta\cdot\omega_z,\, -2\sin\theta\cdot\omega_z,\, 2\omega_\varphi)$, which is non-vanishing for a non-vanishing $\mathbf{L}$; in cartesian coordinates $curl\mathbf{v} = 2(-\omega_\varphi\sin\varphi,\, \omega_\varphi\cos\varphi,\, \omega_z)$. The energy given by (12) reads

$$\frac{\hbar^2 n}{2m}\int d\mathbf{r}\cdot|grad\Phi|^2 = \frac{1}{2m}p_r^2 + \frac{1}{2mr^2}\mathbf{L}^2 \ , \tag{16}$$

and its minimum value is $\Delta = (\pi^2+2)\hbar^2/ma^2$, corresponding to $r = a/\sqrt{2}$ and $l = 1$; it gives 9.6K for the vortex excitation in liquid He^4, in perfect agreement with the experimental data.[20] One can see that the vortices are not defined for a given energy (except for the L_z-component in the wavefunction). In addition, writing up $\Delta = p^2/2\mu$ with $p = \hbar(2\pi/4r) = \hbar(\pi/\sqrt{2}a)$, one gets the effective mass $\mu = 0.2m$ for rotons, in good agreement with the experimental data.[20] It is worth noting that even if L_z is determined, together with the vortex energy, the velocity and its *curl* are not, as a consequence of the quantal nature of the particle microscopic motion; or, conversely, if one allows for an undetermined energy of the vortex, and requires a well-determination of the wavefunction, or of velocity and its *curl*, it is again impossible, due to the quantal nature of the angular momentum components. However, there is one case where the quantal vortex is well defined, and this corresponds to a cylindrical rotator. The phase of the vortex reads then

$$(1/\hbar)\int p_z dr + (1/\hbar)\int L_z d\theta \ , \tag{17}$$

its gradient is given by

$$grad\Phi = \frac{1}{\hbar}(p_z,\, L_z/r) = \frac{m}{\hbar}(v_z,\, r\omega_z) \ , \tag{18}$$

and the energy reads

$$\frac{\hbar^2 n}{2m}\int d\mathbf{r}\cdot|grad\Phi|^2 = \frac{1}{2m}p_z^2 + \frac{1}{2mr^2}L_z^2 \ . \tag{19}$$

The excitation energy diminishes a little (for $L_z = 1$), the roton mass increases slightly, the energy is defined together with the wavefunction, the *curl* of velocity is $2\omega_z$, but it is not defined (actually it vanishes) for a given momentum and energy, since $v_\theta = r\omega_z = L_z/mr$ in that case. Finally it is also worth notingthat the condensate wavefunction is actually a field operator for vortices, as expected for such quantal objects. Also, a rigid body rotates with an angular velocity without conserving the local angular momentum ($v = \omega r$), and the local velocity has a non-vanishing *curl* (2ω), so that it has a rotational flow, in contrast with a superfluid that rotates with a constant distribution of angular momentum ($v = L/mr$), and no *curl* of velocity (potential flow); a classical fluid is capable of both a potential and a rotational flow (as an excited superfluid too), and the extent to which its flow is rotational expresses its resemblance to a rigid body and its developing turbulence.

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