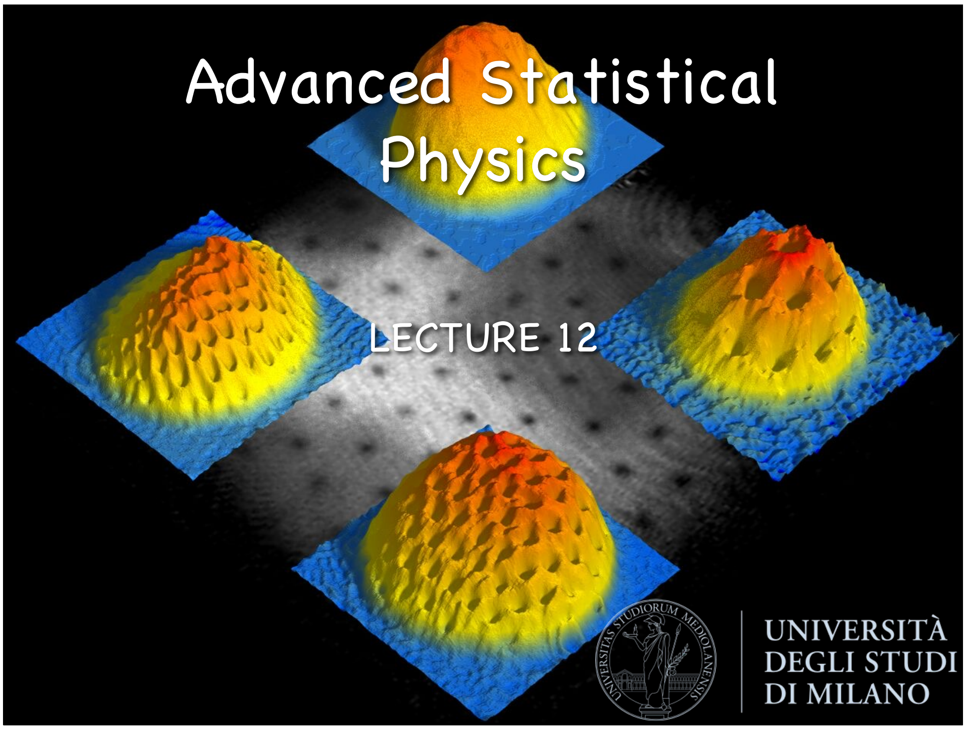

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Outline

- The density matrix in coordinate representation
- Extension of BEC in presence of interaction
- The one-body density matrix
- The weakly interacting Bose gas (WIBG)
- One body density matrix in the ideal and WIBG

- Scope: to formalize the investigation of Bose-Einstein condensation in an interacting system and to start investigate quantum interacting systems

2

2

Density matrix in the coordinate representation

- It is possible to discuss a statistical system in the coordinate representation; we can write the density matrix as

$$\rho(x',x) \overset{def.}{=} \langle x'|\hat{\rho}|x\rangle = \sum_i p_i \langle x'|\phi_i\rangle\langle\phi_i|x\rangle = \sum_i p_i \phi_i^*(x)\phi_i(x')$$

which for a pure state $|\phi_i\rangle$ becomes

$$\rho(x',x) = \phi_i^*(x)\phi_i(x')$$

- In the coordinate representation we write

$$\langle\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) = \int dx \langle x|\hat{\rho}\hat{A}|x\rangle =$$

$$= \int dx dx' \langle x|\hat{\rho}|x'\rangle\langle x'|\hat{A}|x\rangle = \int dx dx' \rho(x,x')\langle x'|\hat{A}|x\rangle$$

- In case A is diagonal in the coordinate representation: A=f(x)

$$\langle f(x)\rangle = \int dx dx' \rho(x,x')\langle x'|f(x)|x\rangle = \int dx dx' \rho(x,x') f(x)\langle x'|x\rangle =$$

$$= \int dx dx' \rho(x,x') f(x)\delta(x-x') = \int dx f(x)\,\rho(x,x)$$

3

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Density sub-matrices

- Consider now operators which consists of a sum of one-body or two body terms; for example an external potential

$\hat{V} = \sum_i u^{(1)}(\vec{r}_i)$, or a two-bodies interaction potential $\hat{V} = \sum_{i<j} u^{(2)}(\vec{r}_i,\vec{r}_j)$

- the statistical average of this kind of operators can be obtained directly by using sub-matrix: we define the one-particle density matrix

$$\rho_1(\vec{r},\vec{r}') = \frac{1}{\mathrm{Tr}(\hat{\rho})}\int d\vec{r}_2 \cdots d\vec{r}_N\, \rho(\vec{r},\vec{r}_2\cdots\vec{r}_N;\vec{r}',\vec{r}_2\cdots\vec{r}_N)$$

in pratica con
fai la traccia
sulle altre N-1 particelle

- And the two-particle density matrix

$$\rho_2(\vec{r}_1\vec{r}_2,\vec{r}_1'\vec{r}_2') = \frac{1}{\mathrm{Tr}(\hat{\rho})}\int d\vec{r}_3 \cdots d\vec{r}_N\, \rho(\vec{r}_1,\vec{r}_2,\vec{r}_3\cdots\vec{r}_N;\vec{r}_1',\vec{r}_2',\vec{r}_3\cdots\vec{r}_N)$$

- It is easy to see that such functions are very useful for the calculation of one-body and two-body properties (diagonal in the coordinate representation), once the degrees of freedom are itinerant and the system is homogeneous and isotropic

4

4

- In fact, consider a one-body property:

$$\left\langle \sum_i u^{(1)}(\vec{r}_i) \right\rangle = \frac{1}{\mathrm{Tr}(\hat{\rho})} \int d\vec{r}_1 \cdots d\vec{r}_N \sum_i u^{(1)}(\vec{r}_i)\; \rho(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N; \vec{r}_1, \vec{r}_2 \cdots \vec{r}_N) =$$

$$= \frac{N}{\mathrm{Tr}(\hat{\rho})} \int d\vec{r}_1\, u^{(1)}(\vec{r}_1) \int d\vec{r}_2 \cdots d\vec{r}_N\;\; \rho(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N; \vec{r}_1, \vec{r}_2 \cdots \vec{r}_N) = N \int d\vec{r}\, u^{(1)}(\vec{r})\, \rho_1(\vec{r}, \vec{r})$$

(this is not surprising … in a future lecture we shall see that $\rho_1(r,r)$ is proportional to the one particle density function $\rho^{(1)}(r)$)

- And, for a two-body property:

$$\left\langle \sum_{i<j} u^{(2)}(\vec{r}_i, \vec{r}_j) \right\rangle = \frac{1}{\mathrm{Tr}(\hat{\rho})} \int d\vec{r}_1 \cdots d\vec{r}_N \sum_{i<j} u^{(2)}(\vec{r}_i, \vec{r}_j)\; \rho(\vec{r}_1, \vec{r}_2, \vec{r}_3 \cdots \vec{r}_N; \vec{r}_1, \vec{r}_2, \vec{r}_3 \cdots \vec{r}_N) =$$

$$= \frac{N(N-1)}{2 \cdot \mathrm{Tr}(\hat{\rho})} \int d\vec{r}_1\, d\vec{r}_2\, u^{(2)}(\vec{r}_1, \vec{r}_2) \int d\vec{r}_3 \cdots d\vec{r}_N\;\; \rho(\vec{r}_1, \vec{r}_2, \vec{r}_3 \cdots \vec{r}_N; \vec{r}_1, \vec{r}_2, \vec{r}_3 \cdots \vec{r}_N) =$$

$$= \frac{N(N-1)}{2} \int d\vec{r}\, d\vec{r}\,'\, u^{(2)}(\vec{r}, \vec{r}\,')\, \rho_2(\vec{r}\vec{r}\,'; \vec{r}\vec{r}\,')$$

(this is not surprising … in a future lecture we shall see that $\rho_2(rr',rr')$ is proportional to the two-particle density function $\rho^{(2)}(r,r')$)

5

5

BEC: definition, origin, occurrence, consequences

- Let's go back to the BEC phenomenon. It seems probable that not all of Einstein's contemporaries were persuaded that the observation of BEC, like that in the ideal Bose gas, had any real physical relevance; they could well have argued that the introduction of even weak interactions would destroy the phenomenon
- Bogoliubov theory of a weakly interacting Bose gas does not provide any example because there the macroscopic occupation of the zero momentum state is assumed from the beginning
- The original argument of Einstein not only assumes the absence of interactions but is restricted to thermal equilibrium
- We would like to be able to generalize the definition of BEC to an interacting system which is not necessarily in equilibrium
- The obvious generalization is, in words, "a macroscopic number of particles occupies a single one-particle state"; let us try to make this more precise and quantitative

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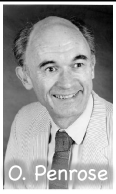


BEC: Penrose and Onsager

In the case of an interacting many-particle system the most useful and generally applicable definition of BEC is the one given by Penrose and Onsager (1956)

- Consider a system with a large number N of bosons characterized by coordinates $\mathbf{r}_i$ (i=1,…,N). It may have arbitrary inter-particle interactions and in addition be subject to an arbitrary single-particle potential, in general time-dependent

- Any pure many-body state s of the system can be written in the form

$$\psi_N^s \equiv \psi_s(\vec r_1, \vec r_2, \cdots, \vec r_N)$$ stato s a N particelle

  where the function ψ_s is symmetric under exchange of any pair i,j.

- Similarly, the most general state of the system can be written as a mixture of different such normalized pure states s with weights p_s

7

7

- Consider now the one-body density matrix defined by the prescription (a factor N is here introduced in the definition):

$$\rho_1(\vec r, \vec r') \equiv N \sum_s p_s \int d\vec r_2\, d\vec r_3 \cdots d\vec r_N \psi_s^*(\vec r, \vec r_2, \cdots, \vec r_N)\psi_s(\vec r', \vec r_2, \cdots, \vec r_N) =$$

$$= \sum_s p_s N \int d\vec r_2\, d\vec r_3 \cdots d\vec r_N \left\langle s \middle| \vec r, \vec r_2, \cdots, \vec r_N \right\rangle \left\langle \vec r', \vec r_2, \cdots, \vec r_N \middle| s \right\rangle =$$

$$= \sum_s p_s \int d\vec r_2\, d\vec r_3 \cdots d\vec r_N \left\langle s \middle| \hat\Psi^+(\vec r) \middle| \vec r_2, \cdots, \vec r_N \right\rangle \left\langle \vec r_2, \cdots, \vec r_N \middle| \hat\Psi(\vec r') \middle| s \right\rangle = \left\langle \hat\Psi^+(\vec r)\hat\Psi(\vec r') \right\rangle$$ media negli stati s

- Thus ρ_1 is proportional to the product among the probability amplitude to have a particular particle at $\mathbf{r}$ times the probability amplitude obtained moving it at $\mathbf{r}'$, averaged over the behaviour of all the other N-1 particles e media anche su tutta la miscela s

- In the second quantization "language" ρ_1 is equal to the probability to destroy a particle in $\mathbf{r}'$ and create it in $\mathbf{r}$

- Note also that:

$$\rho_1(\vec r, \vec r) = \rho_N^{(1)}(\vec r)$$

8

8

- It follows directly from its definition that ρ_1 is hermitian:

$$\rho_1(\vec{r},\vec{r}') \equiv \rho_1^*(\vec{r}',\vec{r})$$

- It then follows that ρ_1 can be diagonalized, i.e. written in the form

$$\rho_1(\vec{r},\vec{r}') = \sum_i n_i \, \chi_i^*(\vec{r}) \, \chi_i(\vec{r}')$$

where the functions $\chi_i(\mathbf{r})$ form a complete orthogonal set. Note that in general both the eigenfunctions χ_i of ρ_1 and its eigenvalues n_i could be functions of time, and that the χ_i certainly need **not** to be eigenfunctions of the single-particle Hamiltonian or indeed of any simple operator, other than ρ_1 itself

sempre gas perché essendo diluiti hanno hamiltoniane semplificabili

- We now state the following definitions:
  1. If all eigenvalues n_i of ρ_1 are of order unity (none of order N), then we say that the system is "normal" (i.e. not Bose-condensed)
  2. If there is exactly one eigenvalue of order N, with the rest of order unity, than we say that the system exhibits "simple BEC"
  3. If there are two or more eigenvalues of order N, with the rest of order unity, then we say it exhibits "fragmented BEC"

definizione generale di BEC anche per gas non ideali

definizione di Penrose Onsager

la maggior parte è condensata in uno stato

condensazione in più stati

9

9

BEC in finite systems

- Strictly speaking phrases like "of order N" and "of order unity" are not quantitatively defined. la definizione di Penrose-Os. ha senso nel l. termodinamico

  quindi sistemi non-finiti

- For certain kinds of systems we can make the definition rigorous by taking an appropriate thermodynamic limit ($N\to\infty$, $V\to\infty$, N/V=cost.); then the statement that some n_i is of "order N" may be defined as equivalent to $n_i/N\to$cost. and "of order unity" means $n_i/N\to 0$

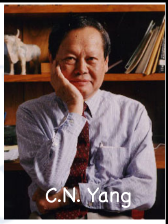
- In various real-life situations (Helium droplets, ultra-cold atomic gas in a trap) there may be no physically meaningful way of taking the thermodynamic limit and hence no rigorous definition of the phrase "of order N"

- However, in such cases there is little difficulty in applying our definitions in a wide sense: consider 10^8 atoms in a trap, and suppose that one eigenvalue of ρ_1 is 5×10^7 and none of the other is greater than 10^3; under these conditions few people would deny that (simple) BEC is occurring

10

10

Off diagonal long range order



- Consider now the single-particle density matrix $\rho_1(\mathbf{r},\mathbf{r}',t)$, but instead of asking explicitly for its eigenvalues, focus on its behaviour in the limit $|\mathbf{r}-\mathbf{r}'|\to\infty$.
- A non zero value of $\rho_1(\mathbf{r},\mathbf{r}',t)$ in this limit is said to correspond to the presence in the system of "off-diagonal long-range order" (ODLRO) (C.N. Yang, 1962)
- Obviously, the correspondence between the previous definition of BEC and the presence of ODLRO in a system obviously cannot be applied in cases such as that of a trapped atomic gas when the limit $|\mathbf{r}-\mathbf{r}'|\to\infty$ cannot be taken … in any case every real system is finite, so don't worry too much about this!
- Consider now what one can obtain via the knowledge of ρ_1 : the one-body density matrix contains information on important physical observables; by setting $\mathbf{r}=\mathbf{r}'$ one finds (on the diagonal) the local density of the system $\rho(\vec r) = \langle \hat\Psi^+(\vec r)\hat\Psi(\vec r)\rangle = \rho_1(\vec r,\vec r)$

- The total number of particles is then: $N = \int d\vec r\, \rho(\vec r) = \int d\vec r\, \rho_1(\vec r,\vec r)$
- The density matrix also determines the momentum distribution:

media di particelle
nello stato $\vec p$

$$n_{\vec p} = \langle a^+_{\vec p} a_{\vec p}\rangle \qquad \left(a_{\vec p} = \int d\vec r\, e^{-\frac{i}{\hbar}\vec p\cdot\vec r}\hat\Psi(\vec r)\right)$$

in fact, one immediately obtains the relation

$$n_{\vec p} = \int d\vec r\, d\vec r'\, e^{\frac{i}{\hbar}\vec p\cdot(\vec r-\vec r')}\langle\hat\Psi^+(\vec r)\hat\Psi(\vec r')\rangle = \int d\vec r\, d\vec r'\, e^{\frac{i}{\hbar}\vec p\cdot(\vec r-\vec r')}\rho_1(\vec r,\vec r') =$$

$$\left[\vec s = \vec r - \vec r';\quad \vec R = (\vec r+\vec r')/2\right] \longrightarrow = \int d\vec R\, d\vec s\, e^{\frac{i}{\hbar}\vec p\cdot\vec s}\rho_1(\vec R+\vec s/2, \vec R-\vec s/2)$$

se non prendo il caso isotropo però anche $n_{\vec p}$ dovrebbe avere termini non diagonali?

- Let us consider the case of a uniform and isotropic system of N particles occupying a volume V in the absence of external potential. In the thermodynamic limit the one-body density matrix depends only on the modulus of the relative variable $\mathbf{s}=\mathbf{r}-\mathbf{r}'$ and one can write

$$\boxed{n_{\vec p} = V\int d\vec s\, e^{\frac{i}{\hbar}\vec p\cdot\vec s}\rho_1(s) \quad ; \quad \rho_1(|\vec r-\vec r'|) = \rho_1(s) = \frac{1}{V(2\pi\hbar)^3}\int d\vec p\, e^{-\frac{i}{\hbar}\vec p\cdot\vec s} n_{\vec p}}$$

- thus ρ_1 and n_p are simply related by a Fourier transform.

- For a normal system the momentum distribution has a smooth behaviour at small momenta and consequently ρ_1 vanishes when **s=r-r'** $\rightarrow\infty$

- The situation is different if instead the momentum distribution exhibits the singular behaviour

$$n_{\vec p} = N_0\delta(\vec p) + \tilde n_{\vec p} \iff \rho(r,r') \not\to 0 \text{ per } |r-r'| \to \infty$$

characterized by a delta function term with a weight N_0 proportional to the total number of particles. This singular term arises from the macroscopic occupation of the single-particle state with momentum **p**=0

- The macroscopic occupation of a single-particle state serves as a general definition of BEC and the quantity $N_0/N\leq 1$ is called the condensate fraction

- By taking the Fourier transform of n_p one finds that, in presence of BEC, the one-body density matrix does not vanish at large distances but approaches a finite value (Off-Diagonal Long-Range Order – ODLRO)

definizione alternativa di BEC in termini di $\rho(r,r')$ $|r-r'| \to \infty$

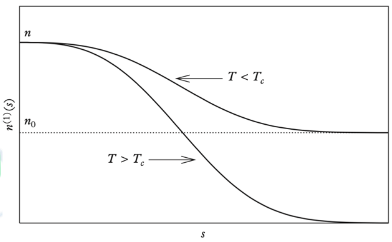
13

13

Off diagonal long range order

$$\rho_1(\vec r,\vec r') = \frac{1}{V(2\pi\hbar)^3}\int d\vec p\, e^{\frac{i}{\hbar}\vec p\cdot(\vec r-\vec r')} n_{\vec p} =$$

$$= \frac{1}{V(2\pi\hbar)^3}\int d\vec p\, e^{\frac{i}{\hbar}\vec p\cdot(\vec r-\vec r')}(N_0\delta(\vec p)+\tilde n_{\vec p}) \xrightarrow[|\vec r-\vec r'|\to\infty]{} \frac{N_0}{V}$$



- The above considerations also hold in presence of interactions which of course affect the value of the condensate density n_0 ; therefore the concept of ODLRO in the one-body density matrix is the required generalization of BEC in presence of interaction between the particles of the system

- While in the ideal gas all the particles are in the condensate at T=0 K i.e. N_0=N, in the presence of interactions one has N_0<N even at T=0 K

- The condensate fraction depends on T and vanishes above T_C where the system exhibits a normal behaviour

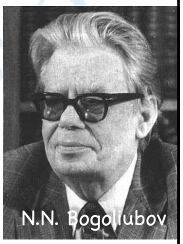
14

14

The weakly interacting Bose gas (WIBG)

non esercitano pressione perché vogliono restare nel g.s

- The previously considered ideal Bose gas is a very peculiar system. It is sufficient to remember that, in the presence of BEC the macroscopic number of particles in the ground state does not contribute to the pressure (infinite compressibility). Therefore it is not surprising that interactions between particles affect the properties of the gas in a dramatic way, even for dilute samples.



- The many-body problem of a weakly interacting collection of Bose particles was solved by Bogoliubov in 1947. His theory is based on a perturbation technique and provides the basis of modern approaches to BEC in dilute gases
- The main feature of the theory is the assumption that a Bose-Einstein condensation occurs at a finite temperature T_C, and that we shall always consider gases at $T<T_C$
- In rarefied gases systems the range r_0 of the interatomic forces is much smaller than the average distance $d=n^{-1/3}$ between particles, fixed by the number density $n=N/V$ of the gas

15

15

quindi come interazione considero solo le collisioni

The Bogoliubov prescription

- This allows us to consider only collisions involving pairs of interacting particles, while collisions among three or more particles simultaneously can be safely neglected più di due particelle vicine poco probabile $\propto n^d$

  n piccolo per i gas

- Assuming pairwise interactions, in the momentum representation, the Hamiltonian reads:

  interazione inv. per traslaz

$$\hat{H} = \sum_{\vec{k}} \frac{\hbar^2 \vec{k}^2}{2m} a^+_{\vec{k}} a_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k},\vec{p},\vec{q}} V_{\vec{q}}\, a^+_{\vec{k}+\vec{q}} a^+_{\vec{p}-\vec{q}} a_{\vec{p}} a_{\vec{k}} \quad \Big| \quad V_{\vec{q}} = \int d\vec{r}\, e^{-\frac{i}{\hbar}\vec{q}\cdot\vec{r}} V(\vec{r}) = V_q$$

(isotropic interaction)

- At low temperatures, a BEC takes place in the k = 0 mode, i.e., in analogy to the ideal Bose gas it is expected that in the ground state the single-particle state with k = 0 is macroscopically occupied: $N_0 \gg 1$
- Hence, we can neglect the interaction of the excited particles with one another and restrict ourselves to the interaction of the excited particles with the condensed particles:

16

16

trascuro le interazioni tra stati eccitati perché debolmente popolati

$$\sum_{\vec k,\vec p,\vec q} V_{\vec q}\, a^+_{\vec k+\vec q} a^+_{\vec p-\vec q} a_{\vec p} a_{\vec k} \cong V_0 a^+_0 a^+_0 a_0 a_0 + \sum_{\vec q\neq 0}^{(\vec p=\vec k=0)} V_{\vec q} a^+_{\vec q} a^+_{-\vec q} a_0 a_0 + \sum_{\vec q\neq 0}^{(\vec p=-\vec k=\vec q)} V_{\vec q} a^+_0 a^+_0 a_{\vec q} a_{-\vec q} + \sum_{\vec p\neq 0}^{(\vec q=\vec k=0)} V_0 a^+_0 a^+_{\vec p} a_{\vec p} a_0 + \sum_{\vec k\neq 0}^{(\vec p=\vec q=0)} V_0 a^+_{\vec k} a^+_0 a_0 a_{\vec k} +$$

$$+ \sum_{\vec q\neq 0}^{(\vec p=\vec q,\vec k=0)} V_{\vec q} a^+_{\vec q} a^+_0 a_{\vec q} a_0 + \sum_{\vec q\neq 0}^{(\vec k=-\vec q,\vec p=0)} V_{\vec q} a^+_0 a^+_{-\vec q} a_0 a_{-\vec q} = V_0 a^+_0 a^+_0 a_0 a_0 + \sum_{\vec k\neq 0}\left[V_{\vec k} a^+_{\vec k} a^+_{-\vec k} a_0 a_0 + V_{\vec k} a^+_0 a^+_0 a_{\vec k} a_{-\vec k} + 2(V_{\vec k}+V_0) a^+_{\vec k} a_{\vec k} a^+_0 a_0\right]$$

- The effect of a_0 and a^+_0 on the state with N_0 particles in the condensate is

$$a_0|N_0,\cdots\rangle = \sqrt{N_0}\,|N_0-1,\cdots\rangle \quad ; \quad a^+_0|N_0,\cdots\rangle = \sqrt{N_0+1}\,|N_0+1,\cdots\rangle$$

- Since N_0 is such a huge number, both of these correspond to multiplication by $\sqrt{N_0}$. Furthermore, it is physically obvious that the removal or addition of one particle from or to the condensate will make no difference to the physical properties of the system. In comparison to N_0, the effect of the commutator $a_0 a^+_0 - a^+_0 a_0 = 1$ is negligible, i.e. the operators a_0 and a^+_0 can be approximated by a number:

$$\boxed{a^+_0 \equiv a_0 \equiv \sqrt{N_0} \cong \sqrt{N}}$$

- This is the so called "Bogoliubov prescription" 17

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17

↳ ovvero quello di stati eccitati non interagenti tra loro

- We must recognize that the term $(a^+_0 a^+_0 a_0 a_0)$ must be worked out with higher accuracy by using

$$N_0 = N - \sum_{\vec k\neq 0} a^+_{\vec k} a_{\vec k} \quad\Rightarrow\quad a^+_0 a^+_0 a_0 a_0 = N_0^2 \cong N^2 - 2N\sum_{\vec k\neq 0} a^+_{\vec k} a_{\vec k}$$

- The Bogoliubov-prescripted Hamiltonian becomes:

$$\boxed{\hat H \cong \sum_{\vec k}\frac{\hbar^2\vec k^2}{2m} a^+_{\vec k} a_{\vec k} + \frac{N^2 \overset{\tilde V(0)}{V_0}}{2V} + \frac{N}{2V}\sum_{\vec k\neq 0} \overset{\tilde V(k)}{V_{\vec k}}\left(a^+_{\vec k} a^+_{-\vec k} + a_{\vec k} a_{-\vec k}\right) + \frac{N}{V}\sum_{\vec k\neq 0} V_{\vec k} a^+_{\vec k} a_{\vec k}}$$

- H is quadratic in a_k and a^+_k and can be diagonalized by the linear transformation

$$\boxed{a_{\vec k} = u_k b_{\vec k} + v_k b^+_{-\vec k} \qquad a^+_{\vec k} = u_k b^+_{\vec k} + v_k b_{-\vec k}}$$

with real symmetric coefficients ($u_k=u_{-k}$; $v_k=v_{-k}$), and with the operators b_k that satisfy Bose commutation relations

$$\left[b_{\vec k}, b_{\vec k'}\right] = \left[b^+_{\vec k}, b^+_{\vec k'}\right] = 0 \quad , \quad \left[b_{\vec k}, b^+_{\vec k'}\right] = \delta_{\vec k,\vec k'}$$

- This is the case when $u_k^2 - v_k^2 = 1$ (canonical transformation)

Proof:

$$\left[a_{\vec k}, a_{\vec k'}\right] = u_k v_{k'}\delta_{\vec k,-\vec k'} - v_k u_{k'}\delta_{\vec k,-\vec k'} = 0$$

$$\left[a_{\vec k}, a^+_{\vec k'}\right] = u_k u_{k'}\delta_{\vec k,\vec k'} - v_k v_{k'}\delta_{\vec k,\vec k'} = (u_k^2 - v_k^2)\delta_{\vec k,\vec k'}$$

18

18

- With the additional calculation step

$$
\begin{aligned}
a^+_{\vec{k}} a_{\vec{k}} &= u_k^2 b^+_{\vec{k}} b_{\vec{k}} + v_k^2 b_{-\vec{k}} b^+_{-\vec{k}} + u_k v_k (b^+_{\vec{k}} b^+_{-\vec{k}} + b_{\vec{k}} b_{-\vec{k}}) \\
a^+_{\vec{k}} a^+_{-\vec{k}} &= u_k^2 b^+_{\vec{k}} b^+_{-\vec{k}} + v_k^2 b_{\vec{k}} b_{-\vec{k}} + u_k v_k (b^+_{\vec{k}} b_{\vec{k}} + b_{-\vec{k}} b^+_{-\vec{k}}) \\
a_{\vec{k}} a_{-\vec{k}} &= u_k^2 b_{\vec{k}} b_{-\vec{k}} + v_k^2 b^+_{\vec{k}} b^+_{-\vec{k}} + u_k v_k (b^+_{-\vec{k}} b_{-\vec{k}} + b_{\vec{k}} b^+_{\vec{k}})
\end{aligned}
$$

… one obtains the following Hamiltonian:

$$
\hat{H} \cong \frac{N^2 V_0}{2V} + \sum_{\vec{k}\neq 0} \left(\frac{\hbar^2 \vec{k}^2}{2m} + \frac{N V_k}{V} \right) \left[u_k^2 b^+_{\vec{k}} b_{\vec{k}} + v_k^2 b_{\vec{k}} b^+_{\vec{k}} + \boxed{u_k v_k (b^+_{\vec{k}} b^+_{-\vec{k}} + b_{\vec{k}} b_{-\vec{k}})} \right] +
$$

$$
+ \frac{N}{2V} \sum_{\vec{k}\neq 0} V_k \left[\boxed{(u_k^2 + v_k^2)(b^+_{\vec{k}} b^+_{-\vec{k}} + b_{\vec{k}} b_{-\vec{k}})} + 2 u_k v_k (b^+_{\vec{k}} b_{\vec{k}} + b_{\vec{k}} b^+_{\vec{k}}) \right]
$$

→ diagonalizzabile se le

where, in order for the non-diagonal terms to disappear, we require that

$$
\left(\frac{\hbar^2 \vec{k}^2}{2m} + \frac{N V_k}{V} \right) u_k v_k + \frac{N V_k}{2V} (u_k^2 + v_k^2) = 0
$$

così determino v_k e u_k

19

19

- Together with $u^2_k - v^2_k = 1$, one now has a system of equations that allow the calculation of u^2_k and v^2_k

- One can write $u_k=\cosh(t_k)$ and $v_k=\sinh(t_k)$, and using the properties $\cosh(2t)=\cosh^2(t)+\sinh^2(t)$, and that $\sinh(2t)=2\cosh(t)\sinh(t)$, one finds

$$
\coth 2t_k = -\frac{\hbar^2 \vec{k}^2 / 2m + nV_k}{nV_k}
$$

- It is convenient to introduce the definition

$$
\varepsilon_k = \left[\left(\hbar^2 \vec{k}^2 / 2m + nV_k \right)^2 - \left(nV_k \right)^2 \right]^{1/2} = \left[\left(\hbar^2 \vec{k}^2 / 2m \right)^2 + \hbar^2 \vec{k}^2 n V_k / m \right]^{1/2}
$$

- The explicit form of the coefficients u_k and v_k turns out to be

$$
u_k = \left[\frac{\left(\hbar^2 k^2 / 2m + nV_k \right) + \varepsilon_k}{2\varepsilon_k} \right]^{1/2} \qquad v_k = -\left[\frac{\left(\hbar^2 k^2 / 2m + nV_k \right) - \varepsilon_k}{2\varepsilon_k} \right]^{1/2}
$$

20

20

- In fact with these definitions one can easily see that $u_k^2 - v_k^2 = 1$ and that

$$u_k v_k = -\left[\frac{\left(\hbar^2\vec{k}^2/2m + nV_k\right)^2 - \varepsilon_k^2}{4\varepsilon_k^2}\right]^{1/2} = -\frac{nV_k}{2\varepsilon_k} \qquad u_k^2 + v_k^2 = \frac{\left(\hbar^2\vec{k}^2/2m + nV_k\right)}{\varepsilon_k}$$

so we recover that

$$\left(\hbar^2\vec{k}^2/2m + nV_k\right)u_k v_k + \frac{nV_k}{2}(u_k^2 + v_k^2) = -\frac{nV_k}{2\varepsilon_k}\left(\hbar^2\vec{k}^2/2m + nV_k\right) + \frac{nV_k}{2}\frac{\hbar^2\vec{k}^2/2m + nV_k}{\varepsilon_k} = 0$$

- The Hamiltonian now has the following diagonalized form

$$\hat{H} \cong \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left(\vec{k}^2/2m + nV_k\right)\left[u_k^2 b_{\vec{k}}^+ b_{\vec{k}} + v_k^2 b_{\vec{k}} b_{\vec{k}}^+\right] + n\sum_{\vec{k}\neq 0} V_k\left[u_k v_k (b_{\vec{k}}^+ b_{\vec{k}} + b_{\vec{k}} b_{\vec{k}}^+)\right] = \cdots$$

… that can be written as (see note-1 in the supplementary material):

$\hat{H} = E_0 + \varepsilon_k \sum b_k^+ b_k$

$$\cdots = E_0 + \sum_{\vec{k}\neq 0} \varepsilon_k b_{\vec{k}}^+ b_{\vec{k}}$$

perché quasi particelle

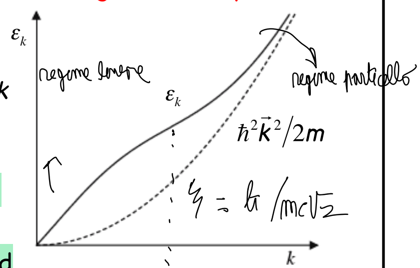
Ground state energy: zero excited quasi-particles

Number of excited quasi-particles of momentum k

idea: le quasi particelle derivano fisicamente dalle eccitazioni per cui le particelle sono fisicamente in $|0\rangle$ ⇒ quindi quando do energia non eccito mai l'una ma una data e l'altra

- The excitation spectrum is given by the famous Bogoliubov dispersion law for the elementary excitations

$$\varepsilon_k = \left[\left(\hbar^2\vec{k}^2/2m\right)^2 + \hbar^2\vec{k}^2 nV_k/m\right]^{1/2} \underset{|\vec{k}|\to 0}{\approx} \hbar k\sqrt{\frac{nV_0}{m}} = c\hbar k$$



- The original system of interacting particles can be therefore described in terms of an Hamiltonian of independent quasi-particles having energy ε_k and whose annihilation and creation operators fulfil Bose commutation rules. The ground state of the interacting system then corresponds to the vacuum of quasi-particles, $b_k|vac\rangle=0$ for any $\mathbf{k}\neq 0$

⇒ quindi le ficcate

- The Bogoliubov theory then predicts that the long wavelength excitations of the interacting Bose gas are sound waves (longitudinal phonons); as we shall see these excitations can also be regarded as the Goldstone modes associated with breaking of "gauge symmetry" caused by BEC. In the opposite limit the dispersion law approaches the free particle law; the transition between the two particle regimes takes places when $\hbar k \approx mc\sqrt{2}$, which corresponds to a characteristic length which is called healing length $\xi = \hbar/mc\sqrt{2}$

però non è lecito solo a N, N_0 grandi?

Some further observations …

- The substitution $a_0^\dagger \equiv a_0 \to \sqrt{N_0}$ cannot be made for a realistic potential since it would results in a poor approximation at short distances, where the potential is strong and quantum correlations are important; it is instead accurate in the case of a soft potential whose perturbation is small at all distances
- The hypothesis $T<T_C$, implies that the relevant values of momenta always satisfy the inequality $pr_0/\hbar \ll 1$; at such momenta the scattering amplitude becomes independent of the scattering angle and can be safely replaced with its low-energy value
- In fact, when a slow (low momentum) particle scatters off a short ranged scatterer, it cannot resolve the structure of the object since its de Broglie wavelength is very long. Therefore to lowest order in energy one has only a spherical symmetric outgoing wave.
- Thus at low density the actual form of the two-body potential is not important to describe the macroscopic properties of the gas, provided that the potential gives the correct value of the s-wave scattering length :

$$a(\vec{q}) = \frac{m}{4\pi\hbar^2}\int d\vec{r}\, e^{-\frac{i}{\hbar}\vec{q}\cdot\vec{r}}\, V(\vec{r}) \underset{q\simeq 0}{\approx} \frac{m}{4\pi\hbar^2}\int d\vec{r}\, V(\vec{r}) = a = \tilde{V}(0)$$

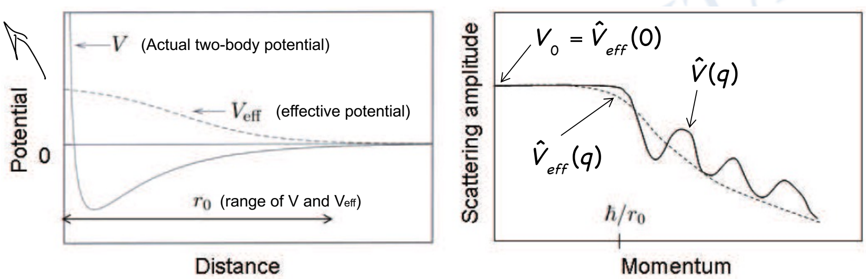
- The condition of diluteness can be written as: $|a|/d = |a|\, n^{1/3} \ll 1$

23

23

però se … con il termine centrifugo

- It is therefore convenient to replace the microscopic potential with an effective potential V_{eff} to which perturbation theory can be safely applied.



- Since only small momenta are involved in the solution of the many-body problem, we are only allowed to consider the q=0 value of the Fourier transform of V_{eff} :

$$V_0 = \int d\vec{r}\, V_{eff}(r) = \frac{4\pi\hbar^2 a}{m}$$

- With this choice the original Hamiltonian reads:

$$\hat{H} = \sum_{\vec{k}} \frac{\vec{k}^2}{2m} a^+_{\vec{k}} a_{\vec{k}} + \frac{V_0}{2V} \sum_{\vec{k},\vec{p},\vec{q}} a^+_{\vec{k}+\vec{q}}\, a^+_{\vec{p}-\vec{q}}\, a_{\vec{p}}\, a_{\vec{k}}$$

24

24

- Note also that by neglecting all terms in the Hamiltonian with nonzero momentum, the “energy” takes the form (no kinetic contribution):

$$E_0 \cong N^2 V_0 / 2V \qquad \left(\cancel{\sum_{\vec{k}} \frac{\vec{k}^2}{2m} a^+_{\vec{k}} a_{\vec{k}}} + \frac{V_0}{2V} \cancel{\sum_{\vec{k},\vec{p},\vec{q}}} \underbrace{a^+_{\vec{k}+\vec{q}} a^+_{\vec{p}-\vec{q}} a_{\vec{p}} a_{\vec{k}}}_{N^2} \right)$$

- The previous equation shows that, contrary to the ideal case, the pressure of a WIBG does not vanish at T=0 K

$$p = -\frac{\partial E_0}{\partial V} = V_0 \frac{n^2}{2}$$

- Accordingly, the compressibility is also finite, and tends to infinity when $V_0 \to 0$

$$\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_{N,T} = -\frac{1}{V}\frac{\partial}{\partial p}\left(N\sqrt{\frac{V_0}{2p}} \right)\Bigg|_{N,T} = \frac{1}{2} n \sqrt{\frac{V_0}{2p^3}} = \frac{1}{V_0 n^2} = \frac{m}{4\pi\hbar^2 a n^2}$$

- The condition of thermodynamic stability implies a positive compressibility, i.e. $a>0$. We then arrive at the important conclusion that a dilute uniform BEC gas can exist only if the s-wave scattering length is positive

OBDM: the ideal Bose gas

- In the non-interacting Bose gas we can easily calculate the off-diagonal one-body density matrix, a key quantity for understanding the nature of long-range order.

- One finds: $$\rho_1(\vec{r},\vec{r}\,') = \left\langle \hat{\Psi}^+(\vec{r})\hat{\Psi}(\vec{r}\,') \right\rangle = \sum_{i,j} \left\langle a_i^+ a_j \right\rangle \varphi_i^*(\vec{r})\varphi_j(\vec{r}\,') =$$

$$= \sum_i \left\langle a_i^+ a_i \right\rangle \varphi_i^*(\vec{r})\varphi_i(\vec{r}\,') = \sum_i n_i\, \varphi_i^*(\vec{r})\varphi_i(\vec{r}\,')$$

where φ_i are the solutions of the free (single) particle eigenvalue Schrödinger equation $H\varphi_i=\varepsilon_i\,\varphi_i$ and n_i are the average occupation number

- therefore the eigenvalues of the one-body density matrix coincide with the solutions of the previous Schrödinger equation and with the corresponding average occupation numbers

- The same property also holds for the ideal Fermi gas and is the consequence of the non-interacting nature of the system

- Using the plane wave solutions for φ_i , we finally obtain the result for $T>T_C$

$$\rho_1(\vec{r}-\vec{r}\,') = \sum_{\vec{p}} \frac{1}{e^{\beta(p^2/2m-\mu)}-1} \frac{e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}}{V} \rightarrow \frac{1}{(2\pi\hbar)^3}\int d\vec{p}\, \frac{e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}}{e^{\beta(p^2/2m-\mu)}-1} \qquad (T>T_C)$$

- And for $T<T_C$ (remember μ=0) by separating the contribution of the condensate (i=0) from that of the thermal component (i≠0)

$$\boxed{\rho_1(\vec{r}-\vec{r}\,') = \frac{N_0(T)}{V} + \frac{1}{(2\pi\hbar)^3}\int d\vec{p}\, \frac{e^{-\frac{i}{\hbar}\vec{p}\cdot(\vec{r}-\vec{r}\,')}}{e^{\beta p^2/2m}-1} \qquad (T<T_c)}$$

where N_0/V is the condensate density.

- Recalling the relationship between the one-body density matrix and the momentum distribution n(**p**) , one can immediately identify the momentum distribution of the ideal Bose gas. In the BEC phase ($T<T_c$) one finds

$$\boxed{n(\vec{p}) = V\int d\vec{s}\,\rho_1(\vec{s})e^{\frac{i}{\hbar}\vec{p}\cdot\vec{s}} = N_0(T)\delta(\vec{p}) + \frac{V}{(2\pi\hbar)^3}\frac{1}{e^{\beta p^2/2m}-1} \qquad (T<T_c)}$$

27

27

while for $T>T_C$ one obtains

$$n(\vec{p}) = \frac{V}{(2\pi\hbar)^3}\frac{1}{e^{\beta(p^2/2m-\mu)}-1} \qquad (T>T_C)$$

The occurrence of the δ function in the momentum distribution for $T<T_C$ is the clear signature of Bose-Einstein condensation

It is interesting to discuss the behaviour of the one-body density matrix at large distances. This is fixed by the low-p behaviour of the momentum distribution;

$$\frac{1}{e^{\beta p^2/2m}-1} \approx \frac{2mk_BT}{p^2}$$

By using the previous expansion, one finds that the one-body density matrix is characterized by the 1/s behaviour (see note-2 in the supplementary material):

$$\rho_1(s) \underset{s>>1}{\approx} \frac{N_0(T)}{V} + \frac{2mk_BT}{(2\pi\hbar)^3} 2\pi\int_0^\pi d\vartheta \sin\vartheta \int_0^\infty dp\, p^2 \frac{e^{-\frac{i}{\hbar}ps\cos\vartheta}}{p^2} = \underset{\left(\int_0^\infty dx \frac{\sin x}{x} = \frac{\pi}{2}\right)}{\cdots} = \frac{N_0(T)}{V} + \frac{1}{\lambda_T^2}\frac{1}{s} \qquad (T<T_C)$$

28

28

- In order to discuss the behaviour of the one-body density above T_C one should instead use the low-p expansion

$$\frac{1}{e^{\beta(p^2/2m-\mu)}-1}=\frac{z}{e^{\beta p^2/2m}-z}\approx\frac{z}{\beta p^2/2m+(1-z)}=\frac{z2mk_BT}{p^2+p_c^2}$$

where $p_c^2=2mk_BT(1-z)$

This yields, via a three-dimensional Fourier transform, the Yukawa-type law (see note-3 in the supplementary material):

$$\rho_1(s)\approx\frac{2\pi(z2mk_BT)}{(2\pi\hbar)^3}\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}dp\,p^2\frac{e^{-\frac{i}{\hbar}ps\cos\theta}}{p^2+p_c^2}=\cdots=\frac{z}{\lambda_T^2}\frac{e^{-p_cs/\hbar}}{s}\qquad(T>T_c)$$

$$\left(\int_0^\infty dx\frac{x\sin x}{x^2+\alpha^2}=\frac{\pi}{2}e^{-\alpha}\right)$$

So, for $T>T_C$ ρ_1 tends to zero within a microscopic distance fixed by $p_c/\hbar$ and only below T_C, due to BEC ($n_0\neq0$), it remains different from zero at macroscopic distances

29

29

OBDM: the weakly interacting Bose gas

- It is important to distinguish between the quasi-particle occupation number

$$N_p\equiv\left\langle b_p^+b_p\right\rangle=\frac{1}{e^{\beta\varepsilon_p}-1}$$

and the particle occupation number $n_p\equiv\left\langle a_p^+a_p\right\rangle$ which is directly related to the particle momentum distribution.

- This can be easily computed by using the Bogoliubov transformation:

$$n_p\equiv\left\langle a_p^+a_p\right\rangle=\left\langle(ub_p^++vb_{-p})(ub_p+vb_{-p}^+)\right\rangle=$$

these terms vanish for states with a definite number of quasi-particles

$$=\left\langle u^2b_p^+b_p+v^2b_{-p}b_{-p}^++uv(b_p^+b_{-p}^++b_{-p}b_p)\right\rangle=$$

$$=u^2\left\langle b_p^+b_p\right\rangle+v^2\left(\left\langle b_p^+b_p\right\rangle+1\right)=v^2+\left\langle b_p^+b_p\right\rangle(u^2+v^2)$$

where we have used $u\equiv u_p$ and $v\equiv v_p$ and that $v_{-p}=v_p$; this holds for $p\neq0$ where u and v are finite.

30

30

- Thus, the number of atoms in the condensate can be calculated through the relation

$$N_0 = N - \sum_{\vec{p}\neq 0} n_{\vec{p}} = N - \sum_{\vec{p}\neq 0} \langle a^+_{\vec{p}} a_{\vec{p}} \rangle = N - \frac{V}{(2\pi\hbar)^3} \int d\vec{p} \left[v_p^2 + \langle b^+_{\vec{p}} b_{\vec{p}} \rangle (u_p^2 + v_p^2) \right]$$

- The interactions in the gas cause the presence of particles with nonzero momentum, even at absolute zero, where $\langle b^+_p b_p \rangle = 0$, due to the v^2 term.

- The condensate density at T=0 K turns out to be (see note-4):

scattering length

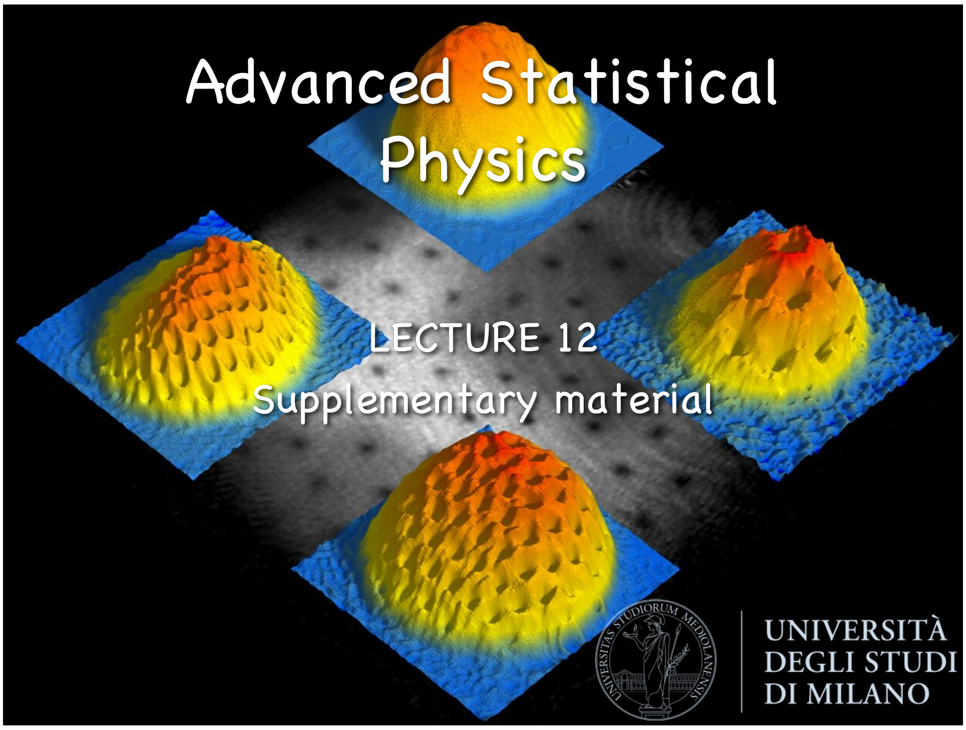
$$\frac{N_0}{V} = \frac{N}{V} - \frac{1}{(2\pi\hbar)^3} \int d\vec{p}\, v_p^2 = n - \frac{1}{(2\pi\hbar)^3} \int d\vec{p} \left[\frac{p^2/2m + mc^2 - \varepsilon_p}{2\varepsilon_p} \right] = \cdots = n \left[1 - \frac{8}{3} \sqrt{\frac{na^3}{\pi}} \right]$$

$$\left(\int_0^\infty dx\, x^2 \left[\frac{x^2+1}{\sqrt{x^4+2x^2}} - 1 \right] = \frac{\sqrt{2}}{3} \right)$$

- This results is very important because we assumed that $|a|\, n^{1/3} \ll 1$; this implies that the condensate fraction at T=0 K is only slightly depressed respect to the 100% value: the Bogoliubov approach is consistent!

Lecture 12: Suggested books

- R. K. Pathria, "Statistical mechanics", II ed., Oxford
- L. Pitaevskii, S. Stringari "Bose Einstein Condensation", Clarendon Press, Oxford



33

Note-1

$(\hbar = 1)$

$$\hat{H} \cong \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left(\vec{k}^2/2m + nV_k\right)\left[u_k^2 b_{\vec{k}}^+ b_{\vec{k}} + v_k^2 b_{\vec{k}} b_{\vec{k}}^+\right] + n\sum_{\vec{k}\neq 0} V_k\left[u_k v_k (b_{\vec{k}}^+ b_{\vec{k}} + b_{\vec{k}} b_{\vec{k}}^+)\right] =$$

$$= \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left(\vec{k}^2/2m + nV_k\right)\left[u_k^2 b_{\vec{k}}^+ b_{\vec{k}} + v_k^2\left(b_{\vec{k}}^+ b_{\vec{k}} + 1\right)\right] + n\sum_{\vec{k}\neq 0} V_k\left[u_k v_k (2 b_{\vec{k}}^+ b_{\vec{k}} + 1)\right] =$$

$$= \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left(\vec{k}^2/2m + nV_k\right)\left[\frac{\left(\vec{k}^2/2m + nV_k\right)}{\varepsilon_k} b_{\vec{k}}^+ b_{\vec{k}} + v_k^2\right] + n\sum_{\vec{k}\neq 0} V_k\left[-\frac{nV_k}{2\varepsilon_k}(2 b_{\vec{k}}^+ b_{\vec{k}} + 1)\right] =$$

$$\begin{cases} u_k^2 + v_k^2 = \dfrac{\left(\vec{k}^2/2m + nV_k\right)}{\varepsilon_k} \\ u_k^2 - v_k^2 = 1 \end{cases} \Rightarrow 2v_k^2 = \frac{\left(\vec{k}^2/2m + nV_k\right)}{\varepsilon_k} - 1 \quad \Rightarrow v_k^2 = \frac{\left(\vec{k}^2/2m + nV_k\right) - \varepsilon_k}{\varepsilon_k}$$

$$= \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left(\vec{k}^2/2m + nV_k\right)\left[\frac{\left(\vec{k}^2/2m + nV_k\right)}{\varepsilon_k} b_{\vec{k}}^+ b_{\vec{k}} + \frac{\left(\vec{k}^2/2m + nV_k\right) - \varepsilon_k}{\varepsilon_k}\right] + n\sum_{\vec{k}\neq 0} V_k\left[-\frac{nV_k}{2\varepsilon_k}(2 b_{\vec{k}}^+ b_{\vec{k}} + 1)\right] =$$

34

34

$$= \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left[\frac{\left(\vec{k}^2/2m + nV_k\right)^2 - \varepsilon_k\left(\vec{k}^2/2m + nV_k\right)}{\varepsilon_k} - \frac{(nV_k)^2}{2\varepsilon_k}\right] + \sum_{\vec{k}\neq 0} b^+_{\vec{k}} b_{\vec{k}}\left[\frac{\left(\vec{k}^2/2m + nV_k\right)^2}{\varepsilon_k} - \frac{(nV_k)^2}{\varepsilon_k}\right] =$$

$$= E_0 + \sum_{\vec{k}\neq 0}\varepsilon_k b^+_{\vec{k}} b_{\vec{k}}\left[\frac{\left(\vec{k}^2/2m + nV_k\right)^2 - (nV_k)^2}{\varepsilon_k^2}\right] = E_0 + \sum_{\vec{k}\neq 0}\varepsilon_k b^+_{\vec{k}} b_{\vec{k}}\left[\frac{\left(\vec{k}^2/2m\right)^2 + 2nV_k\,\vec{k}^2/2m}{\varepsilon_k^2}\right] =$$

$$= E_0 + \sum_{\vec{k}\neq 0}\varepsilon_k b^+_{\vec{k}} b_{\vec{k}}\left[\frac{\varepsilon_k^2}{\varepsilon_k^2}\right] = E_0 + \sum_{\vec{k}\neq 0}\varepsilon_k b^+_{\vec{k}} b_{\vec{k}} \qquad \text{c.v.d.}$$

Note also that:

$$E_0 = \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\left[\frac{\left(\vec{k}^2/2m + nV_k\right)^2 - \varepsilon_k\left(\vec{k}^2/2m + nV_k\right)}{\varepsilon_k} - \frac{(nV_k)^2}{2\varepsilon_k}\right] =$$

$$= \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\frac{1}{\varepsilon_k}\left[\left(\vec{k}^2/2m + nV_k\right)^2 - \varepsilon_k\left(\vec{k}^2/2m + nV_k\right) - (nV_k)^2\right] = \qquad \left(\varepsilon_k \underset{|\vec{k}|>>1}{\approx} \frac{\vec{k}^2}{2m} + nV_k\right)$$

$$\underset{|\vec{k}|>>1}{\approx} \frac{nNV_0}{2} + \sum_{\vec{k}\neq 0}\frac{1}{\varepsilon_k}\left[\left(\vec{k}^2/2m + nV_k\right)^2 - \left(\vec{k}^2/2m + nV_k\right)^2 - (nV_k)^2\right] = \frac{nNV_0}{2} - n^2\sum_{\vec{k}\neq 0}\frac{V_k}{\varepsilon_k} < \infty$$

35

35

Note-2

$$\rho_1(s) \underset{s>>1}{\approx} \frac{N_0(T)}{V} + \frac{2mk_BT}{(2\pi\hbar)^3}2\pi\int_0^\pi d\vartheta\,\sin\vartheta\int_0^\infty dp\,p^2\,\frac{e^{-\frac{i}{\hbar}ps\cos\vartheta}}{p^2} = \cdots = \frac{N_0(T)}{V} + \frac{1}{\lambda_T^2}\frac{1}{s} \qquad (T < T_C)$$

$$\left(\int_0^\infty dx\,\frac{\sin x}{x} = \frac{\pi}{2}\right)$$

$$\int_0^\pi d\vartheta\,\sin\vartheta\;e^{-\frac{i}{\hbar}ps\cos\vartheta} = \frac{2\hbar\sin(ps/\hbar)}{ps}$$

$$\int_0^{+\infty} dp\,\frac{2\hbar\sin(ps/\hbar)}{ps} = \frac{2\hbar}{s}\int_0^{+\infty} d\left(\frac{ps}{\hbar}\right)\frac{\sin(ps/\hbar)}{ps/\hbar} =$$

$$= \frac{2\hbar}{s}\int_0^{+\infty} dx\,\frac{\sin(x)}{x} = \frac{2\hbar}{s}\frac{\pi}{2} = \pi\,\frac{\hbar}{s}$$

$$\rho_1(s) = \frac{N_0(T)}{V} + \frac{2mk_BT}{(2\pi\hbar)^3}2\pi\pi\,\frac{\hbar}{s} = \frac{N_0(T)}{V} + \frac{mk_BT}{2\pi\hbar^2}\frac{1}{s} = \frac{N_0(T)}{V} + \frac{1}{\lambda_T^2}\frac{1}{s}$$

$$\lambda_{\rm th} = \sqrt{\frac{2\pi\hbar^2}{mk_{\rm B}T}}.$$

36

36

Note-3

$$\rho_1(s) \approx \frac{2\pi(z2mk_BT)}{(2\pi\hbar)^3}\int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dp\, p^2 \frac{e^{-\frac{i}{\hbar}ps\cos\theta}}{p^2+p_c^2} = \cdots = \frac{z}{\lambda_T^2}\,\frac{e^{-p_c s/\hbar}}{s} \qquad (T > T_c)$$

$$\left(\int_0^{\infty} dx \frac{x\sin x}{x^2+\alpha^2} = \frac{\pi}{2}e^{-\alpha}\right)$$

$$\int_0^{\pi} d\vartheta \sin\vartheta\; e^{-\frac{i}{\hbar}ps\cos\vartheta} = \frac{2\hbar\sin(ps/\hbar)}{ps}$$

$$\int_0^{+\infty} dp\, \frac{p^2}{p^2+p_c^2}\frac{2\hbar\sin(ps/\hbar)}{ps} = \frac{2\hbar}{s}\int_0^{+\infty} dp\, \frac{p\sin(ps/\hbar)}{p^2+p_c^2} =$$

$$= \frac{2\hbar}{s}\int_0^{+\infty} d\left(\frac{ps}{\hbar}\right) \frac{\sin(ps/\hbar)\, ps/\hbar}{(ps/\hbar)^2+(p_c s/\hbar)^2} =$$

$$= \frac{2\hbar}{s}\int_0^{+\infty} dx\, \frac{x\sin x}{x^2+\alpha^2} = \frac{\pi\hbar}{s}e^{-p_c s/\hbar}$$

$$\rho_1(s) = z\frac{2mk_BT}{(2\pi\hbar)^3}2\pi\pi\,\frac{\hbar}{s}e^{-p_c s/\hbar} = z\frac{mk_BT}{2\pi\hbar^2}\,\frac{e^{-p_c s/\hbar}}{s} = \frac{z}{\lambda_T^2}\,\frac{e^{-p_c s/\hbar}}{s}$$

37

37

Note-4

scattering length

$$\frac{N_0}{V} = \frac{N}{V} - \frac{1}{(2\pi\hbar)^3}\int d\vec{p}\; v_p^2 = n - \frac{1}{(2\pi\hbar)^3}\int d\vec{p}\left[\frac{p^2/2m + mc^2 - \varepsilon_p}{2\varepsilon_p}\right] = \cdots = n\left[1 - \frac{8}{3}\sqrt{\frac{na^3}{\pi}}\right]$$

$$\left(\int_0^{\infty} dx\, x^2\left[\frac{x^2+1}{\sqrt{x^4+2x^2}} - 1\right] = \frac{\sqrt{2}}{3}\right)$$

$$\int d\vec{p}\left[\frac{\frac{p^2}{2m}+nV_0-\sqrt{\left(\frac{p^2}{2m}\right)^2+\frac{p^2nV_0}{m}}}{2\sqrt{\left(\frac{p^2}{2m}\right)^2+\frac{p^2nV_0}{m}}}\right] = 4\pi(2m)^{3/2}\frac{1}{2}\int_0^{\infty} d\left(\frac{p}{\sqrt{2m}}\right)\left(\frac{p}{\sqrt{2m}}\right)^2\left[\frac{\left(\frac{p}{\sqrt{2m}}\right)^2+nV_0-\sqrt{\left(\frac{p}{\sqrt{2m}}\right)^4+2nV_0\left(\frac{p}{\sqrt{2m}}\right)^2}}{\sqrt{\left(\frac{p}{\sqrt{2m}}\right)^4+2nV_0\left(\frac{p}{\sqrt{2m}}\right)^2}}\right] =$$

$$= 2\pi(2m)^{3/2}\int_0^{\infty} d\left(\frac{p}{\sqrt{2m}}\right)\left(\frac{p}{\sqrt{2m}}\right)^2\left[\frac{\left(\frac{p}{\sqrt{2m}}\right)^2+nV_0}{\sqrt{\left(\frac{p}{\sqrt{2m}}\right)^4+2nV_0\left(\frac{p}{\sqrt{2m}}\right)^2}} - 1\right] =$$

$$= 2\pi(2mnV_0)^{3/2}\int_0^{\infty} d\left(\frac{p}{\sqrt{2mnV_0}}\right)\left(\frac{p}{\sqrt{2mnV_0}}\right)^2\left[\frac{\left(\frac{p}{\sqrt{2mnV_0}}\right)^2+1}{\sqrt{\left(\frac{p}{\sqrt{2mnV_0}}\right)^4+2\left(\frac{p}{\sqrt{2mnV_0}}\right)^2}} - 1\right] =$$

$$= 2\pi(2mnV_0)^{3/2}\int_0^{\infty} dx\, x^2\left[\frac{x^2+1}{\sqrt{x^4+2x^2}} - 1\right]$$

$$V_0 = \int d\vec{r}\, V_{eff}(r) = \frac{4\pi\hbar^2 a}{m}$$

$$\Longrightarrow \frac{N_0}{V} = n - \frac{2\sqrt{2}\pi(2mnV_0)^{\frac{3}{2}}}{3(2\pi\hbar)^3} = n\left[1 - \frac{8}{3}\frac{(4\pi)^{\frac{3}{2}}\pi\sqrt{n}\left(\frac{mV_0}{4\pi\hbar^2}\right)^{\frac{3}{2}}}{(2\pi)^3}\right] = n\left[1 - \frac{8}{3}\sqrt{\frac{na^3}{\pi}}\right]$$

38

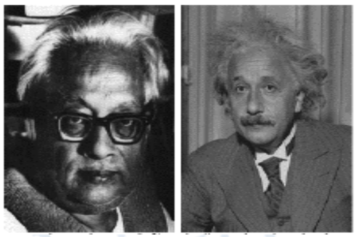
The history of BEC

There are several good reasons to review some of the highlights of the early search for BEC and how we think about it:

- many of the players were among the greatest physicists of the 20th century. Moreover, many of the key concepts of modern physics (elementary excitations, collective modes, broken symmetry, order parameter, etc) were first introduced in dealing with superfluid ^{4}He
- the literature on superfluid ^{4}He has three major rivers which often have little overlap:
  - BEC and a macroscopic wave function : London
  - Many-body wavefunctions for N atoms: Feynman
  - Phenomenological two-fluid theory based on conservation laws and a quasi-particle description: Landau
- The emergence, along this path, of the idea of a macroscopic wavefunction to describe the unique features which arise in "condensed" quantum fluids.

39

Einstein and Bose



- Einstein's famous paper was built on a paper by S.N. Bose in 1924, which gave a novel derivation photon statistics and the Planck distribution. BEC was specifically discussed in the second of three great papers by Einstein on the statistical mechanics of an ideal monatomic gas (written in 25)
- Einstein's paper appeared about a year before the development of quantum mechanics. It was the first time anyone referred to or used de Broglie's new idea of matter waves. Einstein justified applying Bose's calculation using the argument that if particles were waves, they should obey the same statistics as photons. Schrödinger first heard about de Broglie's idea from reading Einstein's paper. So we might say that Schrödinger's wave equation grew out of Einstein's BEC paper, and not the other way around!
- Einstein's work also preceded the concept of Fermi statistics, as well as the division of all particles into two classes (Fermions and Bosons) depending on their net spin
- While the properties of normal Bose gases were extensively studied in the decade after Einstein's 1925 paper, nothing much happened concerning BEC until 1938. Einstein's prediction of a "phase transition" was criticized by arguing it would not occur in a finite system. Second-order phase transitions were not understood yet

40

Fritz London

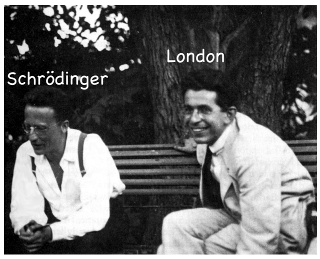
- In the period 1935-37, London (and his brother Heinz London) introduced a new theory of superconductivity based on the of a "macroscopic wave-function". These ideas strongly development of the modern microscopic theory of BCS

- At a major statistical mechanics conference held in Amsterdam in late 1937, London heard discussions which finally clarified the nature of second-order phase transitions (they require the thermodynamic limit $V \rightarrow \infty$ to be defined in a rigorous way). This got London interested in Einstein's forgotten paper on BEC.

- At the same time, London also heard rumors of experimental work showing superfluidity in liquid ^{4}He, below the transition at $T_c \sim 2.17$ K. This transition showed a peak in the specific heat but its physical origin was still a mystery. Indeed, by the early 1930's, there was increasing evidence that below T_c, Helium II behaved in strange ways (sudden absence of boiling below T_c , infinite thermal conductivity, zero viscosity in small channels, etc). London knew ^{4}He was a Boson (S = 0) and immediately put the two ideas together: Some sort of BEC was involved in the strange phase transition shown by superfluid ^{4}He. As evidence, London noted that Einstein's formula for T_{BEC} gave a good estimate of the observed transition temperature and the specific heat of the ideal gas had a peak at T_{BEC}.

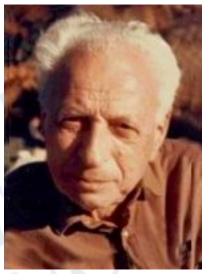
41

- The statistical mechanics Conference in Amsterdam was in November, 1937. In January, 1938, Kapitza and, independently, Allen and Misener, published their key experiments on superfluidity in the same issue of Nature. London had his idea in late January, submitted a one page letter to Nature in early March, which was duly published in April 9, 1938. London discussed his idea with Tisza in late January, who then submitted a brief note to Nature on April 16, which was published on May 21, 1938. We can all admire the short time needed for publication in those days.
- London was never able to develop his idea about BEC in liquid ^{4}He in a quantitative manner. He had a vision of the correct theory but the techniques needed to fill in the details had to wait until the late 1950's, when many-body theory was developed. However, modern microscopic theories of superfluidity and superconductivity basically vindicate London's concepts and philosophy.
- Earlier in his career, London worked with Schrödinger and shared the latter's idea that the wavefunction in quantum mechanics represented something "real". London's thinking about a macroscopic wavefunction that would describe superfluids and superconductors was clearly influenced by this. However, this approach was not consistent with the developing paradigm of the 1930's. The emphasis on operators in quantum mechanics and the resulting de-emphasis in the Copenhagen interpretation on "pictures" made the tentative ideas of London and Tisza seem very old-fashioned



42

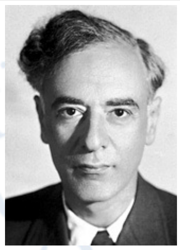
Laszlo Tiza



- Lazlo Tisza worked in Landau's group in Kharkov during 1935-1937. In the period 1937-1938, he was a visiting research fellow at the College de France in Paris, where he interacted with London.
- London told Tisza about this idea and after one restless night, Tisza came up with the two-fluid concept, namely that the Bose condensate acted as a new collective degree of freedom, which could move coherently without friction and hence give rise to superfluid behaviour.
- Tisza had nothing but an ideal Bose gas as a microscopic model, yet he developed a "two-fluid hydrodynamics" based on the notion of a superfluid and normal fluid. Tisza's two long papers published in 1940 on his two-fluid hydrodynamics are very impressive even today. He could explain all the experiments exhibiting superfluidity, usually involving the normal fluid and superfluid moving in opposite directions. Tisza also predicted the existence of a new kind of hydrodynamic oscillation, a temperature wave (later called second sound by Landau).
- London took many years to accept the huge "leap" that Tisza made connecting his BEC idea with superfluid behaviour based on a two-fluid model.

43

L.D. Landau



- In 1941 a paper of Landau on superfluid 4He changed how we think about all condensed matter systems.
- While essentially phenomenological, Landau introduced a "new" hydrodynamics to describe low frequency superfluid phenomena based on the motion of two fluids described by ρ_n, ρ_s, $\mathbf{v}_n$, $\mathbf{v}_s$, many ways similar to those developed earlier by Tisza.
- In addition, Landau also introduced the novel but powerful idea that the liquid could be described in terms of a "gas of weakly interacting quasiparticles", with a relatively simple energy spectrum for two kinds of quasiparticles: phonons and rotons. This quasiparticle idea allowed Landau to do quantitative calculations.
- Landau orginally tried to justify his quasiparticle energy spectrum using "quantum hydrodynamics" but this was never convincing. In a later brief addendum, Landau introduced the now famous phonon-roton spectrum as a single excitation branch. This modified spectrum was deduced using fits to better thermodynamic data which had become available.
- Landau also introduced the idea of collective modes as distinct from quasiparticles (or elementary excitations). In particular, first and second sound are collective modes in the "gas of quasiparticles".

44

- By the early 1950's, the Landau-Khalatnikov (LK) theory had overshadowed the London-Tisza scenario, which still lacked a microscopic model in which interactions between atoms were included. An important event was in 1946, when Peshkov in Moscow succeeded in observing second sound as a temperature oscillation and showed that the temperature dependence of the second sound velocity agreed with the prediction of two-fluid hydrodynamics.
- The direct measurement of the phonon-roton spectrum using inelastic neutron scattering (1959-1961) dramatically confirmed the correctness of the Landau approach. To this day, the LK theory is the standard theory used to describe the properties of superfluid ^{4}He.
- In his landmark paper, however, Landau never mentioned the fact that 4He atoms were Bosons, let alone the existence of a Bose condensate. Indeed, the experimental low temperature community still tends to feel BEC cannot play a very fundamental role since the LK theory hardly mentions it!
- On the other hand, since the 1960's, most theorists have viewed the LK theory as a phenomenological theory whose microscopic basis lies in the existence of a Bose macroscopic order parameter.
- Why did Landau resist the idea of a Bose condensate as being relevant to superfluid ^{4}He? This is strange, since it was Landau himself who in 1937 formulated the usefulness of the concept of an order parameter to deal with second-order phase transitions.
- However, even as late as 1949, Landau wrote a blistering attack on Tisza's work in the Physical Review.

45

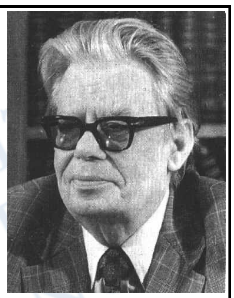
- Landau deeply accepted the Copenhagen view of quantum mechanics. In particular, he accepted that the proper procedure was to take a classical description and quantize it by introducing operators for the physical observables. Thus, Landau believed that the correct way of understanding a "quantum" liquid was to quantize the standard hydrodynamical theory of a "classical" liquid. This is what he tried to do with his "quantum hydrodynamics" (1941) - an approach that never succeeded. However, it suggests why in the 1940's, Landau felt that it was absolutely wrong to try and develop a theory of a "quantum liquid" starting from a "quantum gas"
- In modern renormalization group language, one might say that Landau felt these two systems corresponded to two different fixed points.
- Landau was deeply permeated with the idea that a good theory should be able to give a quantitative explanation of experimental data. He did not like "vague" theories which could not be pushed to a clear experimental conclusion. In any event, as far as I know, Landau never "officially" changed his views of the London program that a theory of superfluid 4He could be developed "starting" from an ideal Bose gas.
- However, Beliaev in 1957 wrote a paper in which he says: "It allows one to suppose that the difference between liquid He and a non-ideal Bose gas is only a quantitative one, and that no qualitatively new phenomena arise in the transition from gas to liquid". A few paragraphs later, Beliaev ends his paper by thanking "L.D. Landau for criticism of the results", as much of a "stamp of approval" as one could expect.

46

The Landau group (1956)

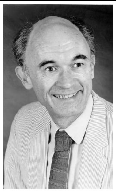
47

N.N. Bogoliubov



- Bogoliubov's paper (1947) showed how BEC was not much altered by interactions in a weakly interacting dilute Bose gas, something which was not obvious at the time.
- However, Bogoliubov showed that interactions completely altered the long wavelength response of a Bose-condensed gas. The predicted phonon spectrum at low momentum was exactly what was assumed by Landau for his quasiparticle dispersion relation and ensured the stability of superfluid flow.
- This paper took up the sputtering program of London and Tisza, and started the developments which led to a "complete" theory by the early 1960's based on the key role of Bose broken symmetry, and how this modified the dynamics of a Bose-condensed system, be it a gas or liquid
- It seems that London never heard of Bogoliubov's work
- Landau clearly recognized the correctness and importance of Bogoliubov's results. However, the paper of Bogoliubov was not "understood" until 1957 or so. This was probably mainly due to the use of second quantization (unfamiliar at that time in condensed matter physics) and the use of a number non-conserving approximation. For example, the famous papers of Feynman as well as those by Lee, Yang and Huang in the middle 1950's make essentially no reference to Bogoliubov's paper.

48



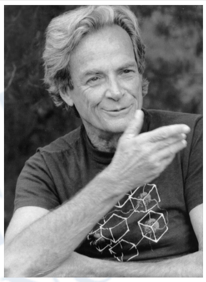
O. Penrose and L. Onsager

- In modern theory, the underlying Bose complex order parameter is $\Phi(\vec{r},t) = \sqrt{n_c(\vec{r},t)}\, e^{i\theta(\vec{r},t)}$

- The superfluid velocity, defined by $m\mathbf{v}_s(\mathbf{r},t) = \hbar\nabla\theta(\mathbf{r},t)$, is easily measured by a variety of experiments. In contrast, the amplitude $\sqrt{n_c}$ is more illusive since it doesn't appear in most measurable properties of superfluid ^{4}He. What is easily studied is the superfluid density ρ_s, which "depends" on n_c but in a "complicated" (unknown) manner.
- In 1956, Penrose and Onsager extended the concept of $\Phi(r)$ to a uniform Bose liquid and discussed the associated long-range correlations it implied, building on earlier work by Penrose.
- They also estimated the value of n_c at T=0 K using a ground state wavefunction due to Feynman and found $n_c \simeq 0.08n$ in liquid ^{4}He. This estimate has not changed much in 50 years! "Convincing" experimental values of n_c were only obtained in early 1980's, using inelastic neutron scattering to extract the momentum distribution of the ^{4}He atoms. These experiments also gave (when carefully analyzed) $n_c \sim 0.1n$ at T=0 K and show that $n_c \to 0$ as $T \to T_c$.

49

R. P. Feynman



- Several brilliant papers by Feynman posed the important question: How are the many-body wavefunctions for the ground state and lowest excited states of liquid 4He effected Bose statistics?
- These papers are essentially variational in nature, but Feynman managed to give the first "microscopic" understanding based on quantum mechanics of the roton part of the quasiparticle spectrum (as first postulated without any explanation by Landau in 1947).
- Feynman's papers were the beginning of a huge literature on various approximations for the wavefunctions of many-particle quantum states. In particular, one should mention the extensive work of Feenberg and his students and co-workers in developing what is called the "correlated basis function" approach. This has been mainly successful in calculating ground-state properties. However, the role of a Bose condensate in all these theories is obscure. It appears, at best, as a sort of "side effect". Little contact is made with the field-theoretic approach based on a macroscopic wave-function.
- Feynman also did fundamental work on vortices and their role in superfluid ^{4}He. In this connection, Feynman's work inadvertently popularized the idea that somehow "rotons" were fundamentally connected to superfluidity - and moreover, these were related to vortices. This is still a lingering belief in parts of the low temperature community, with not much justification! Needless to say, there are vortices in dilute Bose gases but no "rotons".

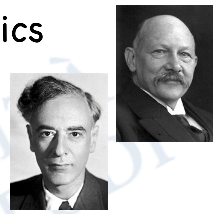
50

The Golden era of BEC

- The "Golden Period" (1957 - 1965) ends our history. In this period, many important theorists attacked the interacting Bose-condensed gas problem.
- However this work, until recently it was largely unknown since it was somewhat uncoupled from experiments on liquid ^{4}He and involved a very complex formalism.
- Out of these efforts came a way of "isolating" the profound role of a condensate on the response functions of a Bose-condensed fluid. These studies often used a weakly interacting dilute Bose gas as an illustration. Thus a huge amount of theoretical insight was gained and a whole literature developed about a "fictitious" system, namely a Bose-condensed gas! Today, more than thirty years later, all this "useless" work is very relevant to trapped atomic gases, apart from the need to add a trapping potential.
- A key development relevant to trapped gases was due to Pitaevskii in the period 1959-61 (Gross-Pitaevskii equation). However, Pitaevskii's real contribution was not this particular equation - rather it lies more in introducing the whole idea of a macroscopic wave-function which could depend on both position and time. This work was no doubt inspired by the use of a similar "wavefunction" by Ginzburg and Landau in their pioneering theory of spatially inhomogeneous superconductors

51

Nobel Prize in "BEC/superfluid" Physics



- 1913 - Heike Kamerlingh Onnes "for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium"
- 1962 - Lev Landau "for his pioneering theories for condensed matter, especially liquid helium"
- 1972 - John Bardeen, Leon N. Cooper, Robert Schrieffer "for their jointly developed theory of superconductivity, usually called the BCS-theory"

- 1973 - Leo Esaki, Ivar Giaever, "for their experimental discoveries regarding tunneling phenomena in semiconductors and superconductors" and Brian D. Josephson "for his theoretical predictions of the properties of a supercurrent through a tunnel barrier, in particular those phenomena which are generally known as the Josephson effects"
- 1974 - Antony Hewish "for his decisive role in the discovery of pulsars"
- 1978 - Pyotr Kapitza "for his basic inventions and discoveries in the area of low-temperature physics"
- 1987 - J. Georg Bednorz, K. Alex Müller "for their important break-through in the discovery of superconductivity in ceramic materials"

52

- 1993 - Russell A. Hulse, Joseph H. Taylor Jr. “for the discovery of a new type of pulsar, a discovery that has opened up new possibilities for the study of gravitation”
- 1996 - David M. Lee, Douglas D. Osheroff, Robert C. Richardson “for their discovery of superfluidity in helium-3”
- 1997 - Steven Chu, Claude Cohen-Tannoudji, William D. Phillips “for development of methods to cool and trap atoms with laser light”
- 2001 - Eric A. Cornell, Wolfgang Ketterle, Carl E. Wieman “for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates”
- 2003 - Alexei A. Abrikosov, Vitaly L. Ginzburg, Anthony J. Leggett “for pioneering contributions to the theory of superconductors and superfluids”
- 2016 – David J. Thouless, F. Duncan M. Haldane and J. Michael Kosterlitz "for theoretical discoveries of topological phase transitions and topological phases of matter"

53