Last lecture (#7):

We discussed Bose-Einstein condensates and considered examples in dilute atomic gases at ultra-low temperatures. Even in these dilute systems, residual interactions cannot be ignored. They lead to modifications of the spectrum of low-lying excitations, to finite Landau critical velocities and to superfluidity.

To go further we need a more microscopic description. This leads us to coherent states for superfluids and the formalism of second quantization. We made a start last time and in this lecture we will develop a Hamiltonian in second quantized form that is central to the study of interacting Bose as well as Fermi systems, and introduce the Bogoliubov theory.

Lecture 8:

I. Creation and Annihilation Operators and Coherent States for Bose Systems
  - IA. Generalization of Harmonic Oscillator Formalism
  - IB. Coherent States for a Bose System

II. Second Quantization Forms of Quantum Fields and Hamiltonian
  - IIA. Kinetic Energy & Quantum Field Operators
  - IIB. Potential Energy, Density Operators & Hamiltonian

III. Introduction to the Bogoliubov Theory

Appendix A: Examples of States of a Bose System in the Schrödinger and Occupation Number Representations

Appendix B: Commutation Rules for Fermions

Literature: Annett chs. 2 & 5, Pethick & Smith chs. 8 & 10, Waldram chs. 2, 9 & appendix

I. Creation and Annihilation Operators and Coherent States for Bose Systems

IA. Generalization of Harmonic Oscillator Formalism

- Photons: the electromagnetic field can be represented in terms of modes with wavevector k, each of which behaves as an oscillator of frequency $\omega = ck$. For each mode we introduce a_k and a_k^+ which annihilate and create, respectively, a photon of wavevector k. For a given k, the commutation rules for these operators are the same as for the lowering and raising operators of a harmonic oscillator. The annihilation and creation operators for different k's all commute.

- More General Bose Systems: the above treatment for massless Bose particles (photons) extends to massive Bose particles when the boson number is not conserved, as in a grand canonical ensemble. All of the properties of the creation and annihilation operators carry over. The form of the single-particle energy spectrum and the (now finite) value of the chemical potential are the main changes.

- The quantum states are described in terms of the occupation numbers in basis states of definite one-particle occupation

$$|n_{k_1}, n_{k_2}, \ldots > \equiv |n_1, n_2, \ldots >$$

The creation operator $a_{k_i}^+$ increases n_i by unity and multiplies the state by $\sqrt{n_i + 1}$

$$a_{k_i}^+ |n_1, n_2, \ldots, n_i, \ldots > = \sqrt{n_i + 1}\, |n_1, n_2, \ldots, n_i + 1, \ldots >$$

Similarly, a_{k_i} reduces n_i by unity and multiplies the state by $\sqrt{n_i}$

$$a_{k_i} |n_1, n_2, \ldots, n_i, \ldots > = \sqrt{n_i}\, |n_1, n_2, \ldots, n_i - 1, \ldots >$$

$$\therefore \quad a_{k_i}^+ a_{k_i} |n_1, n_2, \ldots, n_i, \ldots > = \underbrace{\sqrt{(n_i - 1) + 1}\sqrt{n_i}}_{n_i}\, |n_1, n_2, \ldots, n_i, \ldots >$$

Thus, $\boxed{\hat{n}_k = a_k^+ a_k}$ is the occupation number operator.

All other relations follow in a similar way by analogy to the simple harmonic oscillator model.

- The commutation rules for bosons can be summarized as follows:

$$[a_k, a_{k'}^+] = \delta_{kk'}, \qquad [a_k^+, a_{k'}^+] = [a_k, a_{k'}] = 0$$

- The occupation number formalism is known as second quantization. It automatically includes particle indistinguish-ability. The statistics of the particles is contained in the commutation rules. So far, we have considered only bosons that have the same commutation rules as the ladder operators of a harmonic oscillator. For fermions the commutation rule

$$[A,B] = AB - BA$$

is everywhere replaced by the anticommutation rule

$$\{A,B\} = AB + BA$$

This crucial change incorporates the Pauli exclusion principle.

IB. Coherent States for a Bose System

With the above generalizations we arrive at coherent states of a boson system of the form

$$|\alpha_{k_0}, \alpha_{k_1}, \ldots > \; = e^{-\sum|\alpha_{k_i}|^2/2} exp\left[\sum \alpha_{k_i} a^{+}_{k_i}\right] | vac >$$

Now $|vac>$ is the vacuum state with no bosons present.

In an ideal laser, for example, one of the modes of the electromagnetic field, say k_s, has macroscopic occupation, $< \hat{n}_{k_s} > = |\alpha_{k_s}|^2$, while the others may be ignored.

The application of this coherent state concept to superfluids will be discussed in the next lecture.

II. 2nd Quantized Forms of Quantum Field & Hamiltonian

IIA. Kinetic Energy & Quantum Field Operators

In order to use the 2nd quantization formalism, we need to write the Hamiltonian in terms of creation and annihilation operators (as we did for the simple harmonic oscillator with the corresponding ladder operators). The kinetic energy operator is

$$\hat{T} = \sum_k \varepsilon_k \hat{n}_k$$

Where $\hat{n}_k = a_k^+ a_k$ is the number operator and ε_k is the one-particle energy corresponding to the one-particle basis state φ_k. The expectation value of the kinetic energy is thus $\Sigma_k\ \varepsilon_k < \hat{n}_k >$.

To write the potential energy in 2nd quantized form it is useful to introduce the Fourier transforms of the operators a_k^+ & a_k , i.e., the quantum fields $\hat{\psi}^+(r)$ & $\hat{\psi}(r)$ in a volume V

$$\hat{\psi}^+(r) = \frac{1}{\sqrt{V}} \sum_k e^{-ik\cdot r} a_k^+ \qquad \hat{\psi}(r) = \frac{1}{\sqrt{V}} \sum_k e^{ik\cdot r} a_k$$

$\hat{\psi}^+(r)$ creates a particle in a position eigenstate and $\hat{\psi}(r)$ annihilates a particle in a position eigenstate.

IIB. Potential Energy, Density Operators & Hamiltonian

For a binary interaction, $g(r)$, dependent only on the separation r of the interacting particles we may write the potential energy of the system of identical particles as

$$\mathcal{V} = \frac{1}{2}\sum_{i\neq j} g(r_i - r_j) = \frac{1}{2}\sum_q g_q(\rho_q^* \rho_q - \frac{N}{V}), \quad \text{where}$$

$$g_q = \int_V dr g(r) e^{-iqr}, \quad \rho_q = \frac{1}{\sqrt{V}}\int_V dr n(r) e^{-iqr} \quad \& \quad n(r) = \sum_i \delta(r - r_i)$$

Here g_q is the Fourier transform of $g(r)$ and ρ_q is the Fourier transform of the particle density $n(r)$. To find the 2nd quantized form of the potential energy we replace $n(r)$ by the operator

$$\boxed{\hat{n}(r) = \hat{\psi}^+(r)\,\hat{\psi}(r)}$$

so that $\hat{\rho}_q^+ = \frac{1}{\sqrt{V}}\sum_k a_{k+q}^+ a_k$ and $\hat{\rho}_q = \frac{1}{\sqrt{V}}\sum_{k'} a_{k'-q}^+ a_{k'}$

The operator $a_{k+q}^+ a_k$ annihilates a particle at k and creates a particle at $k+q$. This increases the momentum by $\hbar q$, but does not change the particle number. The sum of such operators over all k represents a collective mode, i.e., a density fluctuation.

From the above density operators and the commutation rules we find that the potential energy operator in 2nd quantized form is

$$\hat{\mathcal{V}} = \frac{1}{2}\sum_q g_q \left(\hat{\rho}_q^+\hat{\rho}_q - \frac{\hat{N}}{V}\right) = \frac{1}{2V}\sum_{kk'q} g_q \; a_{k+q}^+ a_{k'-q}^+ a_{k'} a_k$$

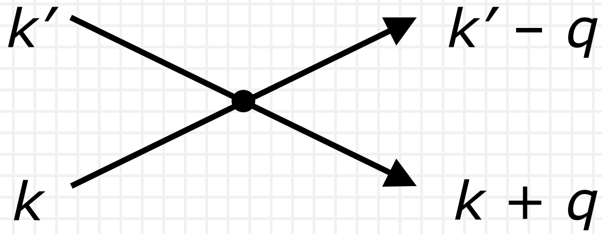
We have used two permutations of the single-particle operators, one of which leads to a constant term that cancels the self-interaction correction term (the term proportional to $\hat{N}/V$). If we use anticommutation rules the sign changes that arise in each permutation cancel out so that this form of $\hat{\mathcal{V}}$ holds for both bosons and fermions. In general we must also include spin indices. Note that if $g(r)$ is a contact interaction

$$g(r) = g\delta(r) \quad \text{then} \quad g_q = g$$

For simplicity we shall use the latter approximation that is expected to be valid for scattering processes in the limit of small momentum transfer $\hbar q$. More general forms of the interaction will be introduced in the final lectures.

Thus, the 2nd quantized form of our model Hamiltonian is

$$\hat{H} = \sum_k \varepsilon_k a_k^+ a_k + \frac{g}{2V} \sum_{kk'q} a_{k+q}^+ a_{k'-q}^+ a_{k'} a_k$$



Including spin indices, this is relevant to, e.g., (i) the Gross-Pitaevskii and Bogoliubov theories for superfluids (bosons, $g > 0$), (ii) the BCS and Bogoliubov theories for conventional superconductors (fermions, $g < 0$ near k_F), & (iii) the Hubbard model for strongly correlated electron systems (e.g., high T_c cuprates).

The kinetic energy is diagonal in the single-particle operators, whereas the potential energy is diagonal in the density operators. One might expect that a superposition of such operators may be needed to diagonalize the full Hamiltonian. This leads us to the Bogoliubov theory.

III. Introduction to the Bogoliubov Theory

If g = 0 the ground state is the simplest BEC state in which all particles are in the same single-particle eigenstate, which we take to be φ_0 (i.e., the k = 0 state). The density of particles n_0 = N_0/V in state φ_0 is then just the total density $n = N/V$. For non-zero but small g we show that the ground state of the Bose system can be approximated by a coherent state (for which, recall, the total number of particles is not fixed). $N_0 = < \hat{N}_0 >$ is now less than $N = < \hat{N} >$ but still macroscopic ($N_0 >> 1$).

Since $N_0 >> 1$, the operators a_0^+ and a_0 effectively commute (the difference between N_0 and N_0+1 being ignorable) and thus become c-numbers, i.e., both can be replaced by $\sqrt{N_0}$

$$a_0^+|\Psi_s\rangle \to \sqrt{N_0}|\Psi_s\rangle, \qquad a_0|\Psi_s\rangle \to \sqrt{N_0}|\Psi_s\rangle$$

In this limit $|\Psi_s>$ is thus approximately an eigenstate of the annihilation operator, and hence approximately a coherent state.

This means the density operator can be approximated as

$$\hat{\rho}_q^+ \rightarrow \frac{1}{\sqrt{V}}(a_q^+ a_0 + a_0^+ a_{-q}) = \sqrt{n_0}(a_q^+ + a_{-q})$$

We have kept terms that dominate as $N_0 \rightarrow \infty$. This is an example of the random phase approximation. Interestingly, a density creation operator in this case reduces to an equal superposition of a particle creation and a particle annihilation operator.

With the above density operator the Hamiltonian reduces to a quadratic form in the single-particle operators* that can be diagonalized by a linear transformation from the starting Bose operators (a_k, a_k^+) to new Bose operators (α_k, α_k^+). The latter correspond to density operators at small *k*, single-particle operators at high *k* and superpositions of both in general.

An excited state can be described in terms of elementary excitations with number density $\alpha_k^+\alpha_k$ and energy E_k. The goal is to find the new Bose operators (α_k, α_k^+) and new excitation energy E_k in terms of the parameters of the Hamiltonian, ε_k & g. This is done via the Bogoliubov transformation.

*We shall use another but equivalent approach in the next lecture.

Appendix A: Examples of States of a Bose System in the Schrödinger and Occupation Number Representations

Let $\{\varphi_k(r)\}$ represent a basis set of one-electron orbitals (ignoring spin for now) and let $|vac> \equiv |0,0,0,\ldots>$ be the vacuum state with no particles. We build up states starting with $|vac>$ via creation operators as follows:

- $a_k^+ \,|\, vac > = \sqrt{1} \times \varphi_k(r) = |\, 0,0,\ldots,(n_k = 1),0,0,\ldots >$

  (The prefactor $\sqrt{n_k + 1} = \sqrt{1}$, since $n_k = 0$ in $|\, vac >$)

- $(a_k^+)^2 \,|\, vac > = \sqrt{2} \times \dfrac{1}{\sqrt{2!}} [\varphi_k(r_a)\varphi_k(r_b) + \varphi_k(r_b)\varphi_k(r_a)]$

  where r_a and r_b are coordinates of particles *a* and *b*, respectively.

- $a_{k'}^+ a_k^+ \,|\, vac > = \sqrt{1} \times \dfrac{1}{\sqrt{2!}} [\varphi_k(r_a)\varphi_{k'}(r_b) + \varphi_k(r_b)\varphi_{k'}(r_a)]$

- $a_k^+ a_k [(a_k^+)^2 \,|\, vac >] = \underbrace{\sqrt{(2-1)+1} \times \sqrt{2}}_{2} \, [(a_k^+)^2 \,|\, vac >]$

- A more complicated example (now including spin in general) might look as follows:

$$|0,2,0,0,1,0,1,0,0,\ldots>$$

$$= \sqrt{\frac{n_1!\,n_2!\ldots}{N!}} \sum_{\text{permutations}} \varphi_2(a)\varphi_2(b)\varphi_5(c)\varphi_7(d) = \frac{\left(a^+_{k_2}\right)^2}{\sqrt{2!}} \frac{\left(a^+_{k_5}\right)}{\sqrt{1!}} \frac{\left(a^+_{k_7}\right)}{\sqrt{1!}} |vac>$$

where $n_2 = 2$, $n_5 = 1$, $n_7 = 1$ (all rest zero) and $N = 4$. In this example we have four identical bosons, two in state 2, one in state 5 and one in state 7. $\varphi_2(a)$, for example, represents a one-particle state in which particle *a* is in state 2 of definite orbit and spin. The sum is over all permutations of the particles (see Waldram, appendix).

Appendix B: Commutation Rules for Fermions

For a system of fermions the many-particle wavefunctions are antisymmetric and are described by Slater determinants. The label k now includes both orbital and spin quantum numbers. Consider, for example, two fermion states with $k' \neq k$

$$a_{k'}^{+} a_{k}^{+} \mid vac > = \frac{1}{\sqrt{2!}} \begin{vmatrix} \varphi_k(a) & \varphi_k(b) \\ \varphi_{k'}(a) & \varphi_{k'}(b) \end{vmatrix}$$

By convention, the new state k' is fed from below in the Slater determinant. Now inverting the creation operators, we get

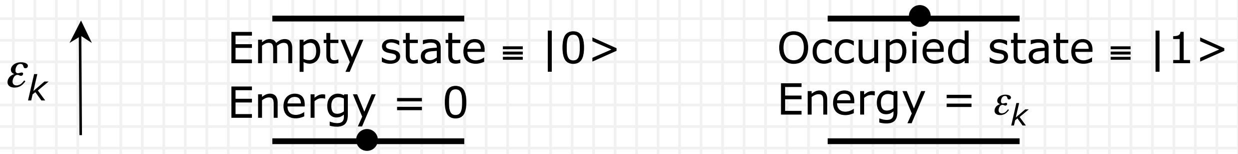
$$a_{k}^{+} a_{k'}^{+} \mid vac > = \frac{1}{\sqrt{2!}} \begin{vmatrix} \varphi_{k'}(a) & \varphi_{k'}(b) \\ \varphi_{k}(a) & \varphi_{k}(b) \end{vmatrix} = -a_{k'}^{+} a_{k}^{+} \mid vac >$$

Thus, the operators for $k \neq k'$ anticommute. Proceeding in this way, we find that the commutation rules for bosons are replaced by analogous anticommutation rules for fermions

$$\{a_k^+, a_{k'}\} = \delta_{kk'}, \qquad \{a_k^+, a_{k'}^+\} = \{a_k, a_{k'}\} = 0$$

The difference in the commutation rules arises from the symmetry properties of the many-particle wavefunctions. The wavefunctions are symmetric for bosons and antisymmetric for fermions.

To demonstrate the commutation rule for a_k^+ and a_k consider the effects of these operators on state k



$a_k|0> = 0$ $\qquad$ $a_k^+|1> = 0$

where |0> means the state is unoccupied (empty) and |1> means it is occupied. Next note that $a_k^+a_k|0> = 0|0>$ and $a_k^+a_k|1> = 1|1>$. This means that $a_k^+a_k$ is the number operator $\hat{n}_k$. Also note that $a_ka_k^+|0> = 1|0>$ and $a_ka_k^+|1> = 0|1>$. This means $a_ka_k^+ = 1 - \hat{n}_k$, i.e., $\{a_k,a_k^+\}=1$ as claimed.

To conclude, creation and annihilation operators anticommute except for products of a_k^+ and $a_{k'}$ for the same state, $k' = k$. Note that the factors $\sqrt{n_k}$ and $\sqrt{n_k + 1}$ that appear in the definitions of a_k and a_k^+ for bosons can only equal zero or one for fermions.

“I remember that when someone had started to teach me about creation and annihilation operators, that this operator creates an electron, I said ‘How do you create an electron? It disagrees with conservation of charge’.”

R.P. Feynman, Nobel Lecture

“In nonrelativistic quantum mechanics the use of second quantization for electron states is purely a matter of notation.”

W.A. Harrison, Solid State Theory

“…the Schrödinger representation has an unnecessary perversity. The particles are actually indistinguishable, but in the Schrödinger representation we first label the particles as though they were distinguishable and then promptly remove the distinguishability by antisymmetrizing the function. It is this antisymmetrization which introduces the algebraic complexity. The occupation number representation, which never labels the particles, is much simpler and more rational in this respect,…”

J.R. Waldram, Superconductivity of Metals and Cuprates

Important reminders:

I) The first supervision for the course will held at the following times (in groups of 4 or 5):

1) 14.00, Friday, 17 February, Mott Seminar Room
2) 15.00, Friday, 17 February, Mott Seminar Room
3) 14.00, Wednesday, 22 February, Committee Room (Room 213, Bragg Building)

II) Because I must attend a scientific meeting on superconductivity in the USA, I would like to hold the last two lectures the week of 5 March, that is:

1) Lecture 11 will be held at 11.00 on Wednesday, 7 March, Mott Seminar Room

   instead of Friday, 24 February
2) Lecture 12 will be held at 11.00 on Friday, 9 March, Mott Seminar Room instead of Wednesday, 29 February

I hope that these changes work for you.

If there are any questions, please see me after the lecture.