III. DILUTE BOSONS: BOGOLIUBOV APPROXIMATION

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In this lecture I briefly review the basics of second quantization and discuss two simple applications. First, I will derive the Hartree-Fock mean-field equation of a dilute Bose gas at finite temperature from a variational principle. Within this approximation, Bose-Einstein condensation is expected exactly at the same critical temperature than an ideal gas at the same density. In order to improve the description of dilute Bosons at low (zero) temperature, we will discuss the Bogoliubov approximation.

A. Reminder on second quantization

Whereas explicit symmetric or antisymmetric wave functions to describe few-body Bose or Fermi systems can be still written down, this description gets lengthy and cumbersome for many-body "bulk" systems. The actual calculation of the partition function of ideal Bose and Fermi gases was much simpler, as only the single particle energies and their occupation number were involved. The formalism of second quantization provides the formal framework for a more compact description basically based on the representation of the wave function in terms of occupation numbers.

1. Creation and annihilation operators

From studying the harmonic oscillator, we should be familiar with creation and annihilation operators which allowed us to construct states of energy n times the fundamental energy $\hbar\omega$ of the oscillator from the state with $n-1$ times that energy. We now describe our many-body wave function by a set of single particle wave functions with corresponding single particle energies ε_k, e.g. the eigenstates and energies of a non-interacting single particle Hamiltonian. A basis for our many-body states can the be build out of states that are simply described by their occupation number, n_k, of each energy level of energy ε_k

$$|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k, \ldots\rangle \tag{1}$$

where $|n_k = 0\rangle$ is simply the empty (vaccum) state. For Bosons, we can now introduce creation and annihilation operators similar to the harmonic oscillator, but for each single particle state, which can be occupied by one or more than particles

$$a_k|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k, \ldots\rangle = \sqrt{n_k}|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k - 1, \ldots\rangle \tag{2}$$

$$a_k^\dagger|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k, \ldots\rangle = \sqrt{n_k + 1}|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k + 1, \ldots\rangle \tag{3}$$

We can explicitly verify that

$$[a_k, a_k^\dagger]_- \equiv a_k a_k^\dagger - a_k^\dagger a_k = 1 \tag{4}$$

and

$$[a_k, a_{k'}^\dagger]_- = \delta_{k,k'}, \quad [a_k, a_{k'}]_- = [a_k^\dagger, a_{k'}^\dagger]_- = 0 \tag{5}$$

as the order of adding or removing particles does not enter for bosons.

For Fermions, we have to consider that only 0 or 1 fermion can occupy one single particle state, so that we have

$$a_k|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k = 1, \ldots\rangle = |\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k = 0, \ldots\rangle \tag{6}$$

$$a_k|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k = 0, \ldots\rangle = 0 \tag{7}$$

$$a_k^\dagger|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k = 0, \ldots\rangle = |\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k = 1, \ldots\rangle \tag{8}$$

$$a_k^\dagger|\varepsilon_1 : n_1, \varepsilon_2 : n_2, \ldots, \varepsilon_k : n_k = 1, \ldots\rangle = 0 \tag{9}$$

and we get anti-commutation relations

$$[a_k, a_k^\dagger]_+ \equiv \{a_k, a_k^\dagger\} \equiv a_k a_k^\dagger + a_k^\dagger a_k = 1 \tag{10}$$

as well as $a_k^2 = (a_k^\dagger)^2 = 0$. Note that the assumption of bosonic commutation relations, Eq. (5), will lead to contradictions. For consistency, we must use anti-commutation rules for the remaining combinations

$$[a_k, a_{k'}^\dagger]_+ = \delta_{k,k'}, \quad [a_k^\dagger, a_{k'}^\dagger]_+ = [a_k, a_{k'}]_+ = 0 \tag{11}$$

The anticommutation expresses that the antisymmetrization of a state with m labels, depend on the order of the m labels. Interchanging two labels will introduce a minus sign. (The basis states in the occupation number representation, Eq. (1), are associated to a Slater determinant for Fermions, whereas the symmetrized states associated for Bosons do not introduce signs.)

2. Field operators

Using creation and annihilation operators, we immediately see that $a_k^\dagger a_k$ gives the number of particles in the state k. Similar, we get simple expressions for all diagonal only involving this occupation number, e.g. the total number of particles in the system, the total energy of a non-interacting system with single particle energies ε_k. Using the corresponding single particle wavefunctions, $\varphi_k(\mathbf{r})$, we can define general field operators

$$\Psi(\mathbf{r}) = \sum_k \varphi_k(\mathbf{r}) a_k \tag{12}$$

$$\Psi^\dagger(\mathbf{r}) = \sum_k \varphi_k^*(\mathbf{r}) a_k^\dagger \tag{13}$$

which satisfy

$$[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_\mp = \delta(\mathbf{r} - \mathbf{r}'), \quad [\Psi(\mathbf{r}), \Psi(\mathbf{r}')]_\mp = [\Psi^\dagger(\mathbf{r}), \Psi^\dagger(\mathbf{r}')]_\mp = 0 \tag{14}$$

where we have used the completeness of single particle states $\sum_k \varphi_k^*(\mathbf{r})\varphi_k(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')$. The operator $\Psi(\mathbf{r})$ and $\Psi^\dagger(\mathbf{r})$ simply describe the annihilation and creation of a particle at position $\mathbf{r}$, and

$$|\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle = \frac{1}{\sqrt{N!}} \Psi^\dagger(\mathbf{r}_N) \cdots \Psi^\dagger(\mathbf{r}_2)\Psi^\dagger(\mathbf{r}_1)|0\rangle \tag{15}$$

is the state of N particles with one at $\mathbf{r}_1$, one at $\mathbf{r}_2$, etc.

A general N-body wave function can then be build via

$$|\Phi\rangle = \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N \varphi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|\mathbf{r}_1 \ldots, \mathbf{r}_N\rangle \tag{16}$$

with

$$\langle \mathbf{r}_1' \ldots, \mathbf{r}_N'|\phi\rangle = \frac{1}{N!} \sum_P (\pm)^P \varphi(\mathbf{r}_{P(1)}', \ldots, \mathbf{r}_{P(N)}') \tag{17}$$

is properly (anti)symmetrized.

3. Operators in second quantization

Since field operators provide a simple tool to manipulate matrix elements in the occupation number representation, it is useful to express the general operators in terms of field operators. The expressions are rather intuitive, the proofs can be found in any quantum mechanics text book. The density of particles at $\mathbf{r}$ is given by

$$\rho(\mathbf{r}) = \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}) \tag{18}$$

since the definition of the field operators above, merely presents a change of the basis vectors of single particle states from k to $\mathbf{r}$.

Similar, the kinetic energy is given in terms of free-particle (plane-wave) states

$$T = \sum_k \frac{k^2}{2m} a_k^\dagger a_k \tag{19}$$

which can be written as

$$T = -\frac{1}{2m}\int d\mathbf{r}\Psi^\dagger(\mathbf{r})\nabla^2\Psi(\mathbf{r}) = \frac{1}{2m}\int d\mathbf{r}[\nabla\Psi^\dagger(\mathbf{r})][\nabla\Psi(\mathbf{r})] \tag{20}$$

The potential energy is diagonal in position space, and we have

$$V = \frac{1}{2}\int d\mathbf{r}_1 \int d\mathbf{r}_2 v(r_1 - r_2)\rho(\mathbf{r}_1)\rho(\mathbf{r}_2) - \frac{\lim_{\epsilon\to 0} v(\epsilon)}{2}\int \rho(\mathbf{r}) \tag{21}$$

which gives

$$V = \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}'\, v(r - r')\Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r}')\Psi(\mathbf{r}')\Psi^\dagger(\mathbf{r}) \tag{22}$$

Note that the order of the operators is important.

B. Bogoliubov approximation

Up to now, we have essentially approximated the state of the system by an essentially non-interacting one, the interaction was treated within a mean-field approximation. In particular at zero temperature, we described the system by a pure condensate – all particles occupied the same single particle state, $k = 0$ for a homogeneous system; within this ansatz, the occupation of this state N_0 is always equal to N. Let us look at the interaction energy again, this time in Fourier space,

$$V = \frac{g_0}{2\mathcal{V}} \sum_{\mathbf{p},\mathbf{k},\mathbf{q}} a^\dagger_{\mathbf{p}-\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}} a_{\mathbf{p}} \tag{23}$$

using a pseudo-potential in Fourier space as discussed previously. Since $N_0 = a_0^\dagger a_0$ is expected to be the only occupation which is extensive, we have $a_k \sim a_k^\dagger \sim N^{-1/2} a_0$ for $k \neq 0$, and we keep only terms which contain condensate operators

$$V \approx \frac{g_0 N_0^2}{2\mathcal{V}} + \frac{g_0}{2\mathcal{V}} \sum_{\mathbf{k}\neq 0} \left[2a^\dagger_{\mathbf{k}} a_{\mathbf{k}} N_0 + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} a_0 a_0 + a_0^\dagger a_0^\dagger a_{\mathbf{k}} a_{-\mathbf{k}} \right] \tag{24}$$

The total Hamiltonian then writes

$$H = \frac{g_0 N_0^2}{2\mathcal{V}} + \sum_{\mathbf{k}\neq 0} \left[\frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{g_0}{\mathcal{V}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} N_0 \right] + \frac{g_0}{2\mathcal{V}} \sum_{\mathbf{k}\neq 0} \left[a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} a_0 a_0 + a_0^\dagger a_0^\dagger a_{\mathbf{k}} a_{-\mathbf{k}} \right] \tag{25}$$

Let us now introduce new operators $b_{\mathbf{k}}$ and $b^\dagger_{\mathbf{k}}$ in order to diagonalize the Hamiltonian.

Let us sketch first the various steps.

- Frequently, a_0 is replaced by the number $\sqrt{N_0}$ in the Hamiltonian. This step violates particle number conservation of the Hamiltonian. It is not difficult to avoid this step, e.g. we can write the kinetic energy of non-condensed particles as

$$\sum_{\mathbf{k}\neq 0} \frac{k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} = \sum_{\mathbf{k}\neq 0} \frac{k^2}{2mN_0} a^\dagger_{\mathbf{k}} a_0 a_0^\dagger a_{\mathbf{k}} + O(1/N) \tag{26}$$

  Introducing $\tilde{a}^\dagger_{\mathbf{k}} = a^\dagger_{\mathbf{k}} a_0/\sqrt{N_0}$, we obtain

$$H = \frac{g_0 N_0^2}{2\mathcal{V}} + \sum_{\mathbf{k}\neq 0} \left[\frac{k^2}{2m} \tilde{a}^\dagger_{\mathbf{k}} \tilde{a}_{\mathbf{k}} + \frac{g_0 N_0}{\mathcal{V}} \tilde{a}^\dagger_{\mathbf{k}} \tilde{a}_{\mathbf{k}} \right] + \frac{g_0 N_0}{2\mathcal{V}} \sum_{\mathbf{k}\neq 0} \left[\tilde{a}^\dagger_{\mathbf{k}} \tilde{a}^\dagger_{-\mathbf{k}} + \tilde{a}_{\mathbf{k}} \tilde{a}_{-\mathbf{k}} \right] \tag{27}$$

  with the same commutation relation to leading order, $[\tilde{a}_{\mathbf{k}}, \tilde{a}^\dagger_{\mathbf{k}}] = 1 + \mathcal{O}(1/N)$. In the following we drop the distinction between $a_{\mathbf{k}}$ and $\tilde{a}_{\mathbf{k}}$.

- We can rewrite the Hamiltonian in the form

$$H = C + \sum_{\mathbf{k}>0} (a^\dagger_{\mathbf{k}} \;\; a_{-\mathbf{k}}) \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a^\dagger_{-\mathbf{k}} \end{pmatrix} \tag{28}$$

  We therefore want to diagonalize the matrix under the constraint that the new basis, a linear combination of $a_{\mathbf{k}}$ and $a^\dagger_{-\mathbf{k}}$, remain bosonic creation and annihilation operators.

- Therefore, we introduce new operators $b_{\mathbf{k}}$ as linear superpositions of $a_{\mathbf{k}}$ and $a^\dagger_{-\mathbf{k}}$

$$b_{\mathbf{k}} = B_k \left(a_{\mathbf{k}} - A_k a^\dagger_{-\mathbf{k}} \right) \tag{29}$$

  where A_k and B_k are real and depend only on $k = |\mathbf{k}|$. We then have

$$a_{\mathbf{k}} = \frac{1}{B_k(1-A_k^2)} \left(b_{\mathbf{k}} + A_k b^\dagger_{-\mathbf{k}} \right) \tag{30}$$

- Imposing the condition $[b_{\mathbf{k}}, b^\dagger_{\mathbf{k}}] = 1 + \mathcal{O}(1/N)$ we can fix B_k.

- Writing the Hamiltonian in terms of $b_{\mathbf{k}}$ we obtain the following form

$$H = C_0 + \sum_{\mathbf{k}\neq 0} \left[C_1(k) + C_2(k) b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + C_3(k) \left(b^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} + b_{\mathbf{k}} b_{-\mathbf{k}} \right) \right] \tag{31}$$

  This Hamiltonian is diagonalized by setting $C_3(k) \equiv 0$ and $C_2(k) \geq 0$ to obtain positive excitation energies. From these conditions we can determines A_k.

Explicitelty, this will give $B_k = (1-A_k^2)^{-1/2}$, and the Hamiltonian writes

$$\begin{aligned} H = {} & \frac{g_0 N^2}{2\mathcal{V}} + \sum_{\mathbf{k}\neq 0} \frac{1}{1-A_k^2} \left[\left(\frac{k^2}{2m} + g_0 n \right) A_k^2 + g_0 n A_k \right] \\ & + \sum_{\mathbf{k}\neq 0} \frac{1}{1-A_k^2} \left[\left(\frac{k^2}{2m} + g_0 n \right) (1 + A_k^2) + 2 g_0 n A_k \right] b^\dagger_{\mathbf{k}} b_{\mathbf{k}} \\ & + \sum_{\mathbf{k}\neq 0} \frac{1}{1-A_k^2} \left[\left(\frac{k^2}{2m} + g_0 n \right) A_k + \frac{g_0 n}{2} (1 + A_k^2) \right] \left[b^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} + b_{\mathbf{k}} b_{-\mathbf{k}} \right] \end{aligned} \tag{32}$$

where $n = N/V$ is the density. We can now eliminate the off diagonal terms in the last line choosing

$$\left(\frac{k^2}{2m} + g_0 n \right) A_k + \frac{g_0 n}{2} (1 + A_k^2) = 0 \tag{33}$$

$$A_k^2 + \frac{2}{g_0 n} \left[\frac{k^2}{2m} + g_0 n \right] A_k + 1 = 0 \tag{34}$$

or

$$A_k = \frac{1}{g_0 n} \left[-\frac{k^2}{2m} - g_0 n \pm \sqrt{\left(\frac{k^2}{2m} + g_0 n \right)^2 - (g_0 n)^2} \right] \tag{35}$$

$$= -x - 1 \pm \sqrt{x(x+2)}, \quad x \equiv \frac{k^2}{2 m g_0 n} \tag{36}$$

We then have

$$\begin{aligned} \left[1 - A_k^2\right]^{-1} &= \left[1 - (x+1)^2 - x(x+2) \pm 2(x+1)\sqrt{x(x+2)} \right]^{-1} = \left[-2x(x+2) \pm 2(x+1)\sqrt{x(x+2)} \right]^{-1} \\ &= \frac{-2x(x+2) \mp 2(x+1)\sqrt{x(x+2)}}{4x^2(x+2)^2 - 4(x+1)^2 x(x+2)} = \frac{-2x(x+2) \mp 2(x+1)\sqrt{x(x+2)}}{-4x(x+2) + [(4x^4 + 16x^3 + 16x^2) - (4x^4 + 16x^3 + 16x^2)]} \end{aligned} \tag{37}$$

The coefficient in front of $b_k^\dagger b_k$ must be positive, since excitation energies must be positive for the ground state energy. In particular for $k \to 0$, since implies that $1 - A_k^2$ must be positive, which can only be true if we chose the positive sign in front of the square root, in A_k, Eq. (36). We therefore have

$$\left[1 - A_k^2\right]^{-1} = \frac{2x(x+2) \pm 2(x+1)\sqrt{x(x+2)}}{4x(x+2)} = \frac{1}{2} + \frac{(x+1)\sqrt{x(x+2)}}{2x(x+2)} \tag{38}$$

Resubstituting, we get for the Hamiltonian

$$H = E_0 + \sum_{\mathbf{k}\neq 0} \omega_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \tag{39}$$

where E_0 is the ground state. Explicitly, we get

$$\omega_k = \sqrt{\frac{k^2}{2m}\left[\frac{k^2}{2m} + 2g_0 n_0\right]} \tag{40}$$

where $n_0 = N_0/V = n + \mathcal{O}(\infty/\mathcal{N})$ which gives a linear (sound-wave) spectrum at small k, and a free particle behavior at large momenta. Further

$$E_0/N = \frac{g_0 n}{2} - \frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left[\frac{k^2}{2m} + g_0 n - \omega_k\right] \tag{41}$$

Notice that the summation on the rhs does not converge for large k since

$$\omega_k = \frac{k^2}{2m}\left[1 + \frac{4mg_0 n}{k^2}\right]^{1/2} \simeq \frac{k^2}{2m}\left[1 + \frac{1}{2}\frac{4mg_0 n}{k^2} - \frac{1}{4}\left(\frac{4mg_0 n}{k^2}\right)^2 + \cdots\right] = \frac{k^2}{2m} + g_0 n - \frac{2mg_0^2 n^2}{k^2} + \cdots, \quad k \to \infty \tag{42}$$

However, notice that we cannot use a simple constant g_0 for the bare potential but rather

$$g_0 = \frac{g}{1 - Cak_c} \simeq g\left[1 + \frac{g}{V}\sum_{\mathbf{q}\neq 0}\frac{4m}{q^2}\right] \tag{43}$$

and the divergence is cancelled by using $g_0 n/2$ up to second order in $g \sim a$ where a is the physically relevant scattering length. The ground state energy then writes

$$E_0/N = \frac{2\pi a n}{m}\left[1 + \frac{128}{15}\sqrt{na^3/\pi}\right] \tag{44}$$

The non-condensed number of particles is given by

$$n' = \frac{1}{V}\sum_{\mathbf{k}\neq 0}\langle 0|a_{\mathbf{k}}^\dagger a_{\mathbf{k}}|0\rangle_B \tag{45}$$

where the Bogoliubov vacuum $|0\rangle_B$ is determined by

$$b_{\mathbf{k}}|0\rangle_B = 0 \tag{46}$$

Therefore, we get

$$n' = \frac{1}{V}\sum_{\mathbf{k}\neq 0}\frac{1}{1 - A_k^2}\langle 0|\left(b_{\mathbf{k}}^\dagger + A_k b_{-\mathbf{k}}\right)\left(b_{\mathbf{k}} + A_k b_{-\mathbf{k}}^\dagger\right)|0\rangle_B = \frac{1}{V}\sum_{\mathbf{k}\neq 0}\left[\frac{A_k^2}{1 - A_k^2} + \frac{1 + A_k^2}{1 - A_k^2}\langle 0|b_{\mathbf{k}}^\dagger b_{\mathbf{k}}|0\rangle_B\right] \tag{47}$$

where we have used the commutation relation. At zero temperature, the last term vanishes and we can evaluate the summation (which is finite since $A_k \sim 1/k^2$ for large k). We get

$$n' = n\frac{8}{3}\sqrt{na^3/\pi} \tag{48}$$

so that even at zero temperature not all particles are in the condensate

$$n_0/n = 1 - n'/n = 1 - \frac{8}{3}\sqrt{na^3/\pi} \tag{49}$$

The Bogoliubov vacuum $|0\rangle_B$ is given by

$$b_{\mathbf{k}}|0\rangle_B = 0 \tag{50}$$

Since we have

$$b_{\mathbf{k}} \sim a_0^\dagger a_{\mathbf{k}} - A_k a_{-\mathbf{k}}^\dagger a_0 \tag{51}$$

the structure of the vaccum is given by

$$|0\rangle_B \sim \left[a_0^\dagger a_0^\dagger - \sum_{\mathbf{k}\neq 0} A_k a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger\right]^{N/2} |0\rangle \tag{52}$$

in leading order $N_0 \sim N$ as can be verified directly. The many-body wave function is then represented by a Jastrow function in position space

$$\Psi_N(\mathbf{r}_1, \ldots, \mathbf{r}_N) \sim \prod_{i<j}[1 + f(r_{ij})] \tag{53}$$

where $f(r) \sim \sum_{\mathbf{k}} A_k e^{i\mathbf{k}\cdot\mathbf{r}}$. Since $A_k \sim g/k^2$ for large k we recover the a/r divergences of the s-wave two-body wave function at small distances.

At finite temperature, the Bogoliubov modes are thermally occupied

$$\langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}}\rangle = \frac{1}{e^{\omega_k/T} - 1} \tag{54}$$

and the non-condensed fraction of particles will grow monotonously with increasing temperature, T, unless $n' = n$ and the normal, non-condensed, state with $n_0 = 0$ is reached. However, close to the critical temperature, the validity of the Bogoliubov approximation breaks down, and corrections have to be included to describe the transition correctly.