7.1 Operator Identity for Gaussian Theories

General case. To form some intuition, let's start with the proof

$$\langle e^{\sum_j b_j x_j}\rangle = e^{\frac{1}{2}\sum_{i,j} b_i \langle x_i x_j\rangle b_j}, \tag{1}$$

with averaging defined as

$$\langle f\rangle = \frac{1}{Z}\int D(\boldsymbol{x}) f(\boldsymbol{x}) e^{-\frac{1}{2}\boldsymbol{x}^{\mathrm{T}} G^{-1}\boldsymbol{x}}, \qquad D(x) = \prod_n dx_n,$$

with $Z = \sqrt{\det(2\pi G)}$ so that $\langle 1\rangle = 1$. Both parts of the (1) could be calculated directly:

$$\langle e^{\sum_j b_j x_j}\rangle = \frac{1}{Z}\int D(x) e^{-\frac{1}{2}\boldsymbol{x}^{\mathrm{T}} G^{-1}\boldsymbol{x} + \boldsymbol{b}\boldsymbol{x}} = \frac{1}{Z}\int D(\boldsymbol{x}) e^{-\frac{1}{2}(\boldsymbol{x}-G\boldsymbol{b})^{\mathrm{T}} G^{-1}(\boldsymbol{x}-G\boldsymbol{b})} e^{\frac{1}{2}\boldsymbol{b}^{\mathrm{T}} G\boldsymbol{b}},$$

and with $\boldsymbol{x}' = \boldsymbol{x} - G\bar{b}$ and $D(\boldsymbol{x}') = D(\boldsymbol{x})$

$$\langle e^{\boldsymbol{b}\boldsymbol{x}}\rangle = \frac{1}{Z}\int D(\boldsymbol{x}') e^{-\frac{1}{2}\boldsymbol{x}'^{\mathrm{T}} G^{-1}\boldsymbol{x}'} e^{\frac{1}{2}\boldsymbol{b}^{\mathrm{T}} G\boldsymbol{b}} = e^{\frac{1}{2}\boldsymbol{b}^{\mathrm{T}} G\boldsymbol{b}} = e^{\frac{1}{2}\sum_{i,j} b_i\langle x_i x_j\rangle b_j},$$

with proved in the previous homework fact that $\langle x_i x_j\rangle = G_{ij}$.

Special case. We want to prove the operator identity

$$\langle e^{i(\varphi(r)-\varphi(0))}\rangle = e^{-\frac{1}{2}\langle(\varphi(r)-\varphi(0))^2\rangle}. \tag{2}$$

With $b(r') = i\delta(r'-r) - i\delta(r')$:

$$\sum_j b_j\varphi_j = \int b(r')\varphi(r')\,dr' = i(\varphi(r)-\varphi(0)),$$

and for other part $\sum_{i,j} b_i\langle x_i x_j\rangle b_j = \langle\sum_{i,j} b_i x_i x_j b_j\rangle$, so

$$\sum_{i,j} b_i x_i x_j b_j = \int b(r')\varphi(r')\varphi(r'')b(r'')\,dr'\,dr'' = \left(\int b(r')\varphi(r')\,dr'\right)^2 = -(\varphi(r)-\varphi(0))^2,$$

thus we proved (2) using (1).

Wick's theorem. Note that from (1) are convenient to obtain Wick's theorem maybe. Expanding (1) in the Taylor series we have from the LHS

$$\langle e^{\sum_j b_j x_j}\rangle = 1 + \frac{1}{2!}\sum_{i,j} b_i b_j\langle x_i x_j\rangle + \frac{1}{4!}\sum_{i,j,k,l} b_i b_j b_k b_l\langle x_i x_j x_k x_l\rangle + \ldots$$

and from the RHS

$$e^{\frac{1}{2}\sum_{i,j} b_i\langle x_i x_j\rangle b_j} 1 + \frac{1}{2}\sum_{i,j} b_i b_j\langle x_i x_j\rangle + \sum_{i,j,k,l} b_i b_j b_k b_l\langle x_i x_j\rangle\langle x_k x_l\rangle + \ldots,$$

so collecting terms with proper B^4 we get

$$\langle x_i x_j x_k x_l\rangle = \langle x_i x_j\rangle\langle x_i x_k\rangle\langle x_j x_l\rangle + \langle x_i x_l\rangle\langle x_j x_k\rangle.$$

This result is known as Wick's theorem.

7.2 Bogoliubov theory

1. Hamiltonian. Consider a microscopic Hamiltonian for bosons with weak contact interactions:

$$\hat{H} - \mu \hat{N} = \sum_p (\varepsilon_p - \mu) \hat{a}_p^\dagger \hat{a}_p + \frac{\varphi}{2V} \sum_{p,p',q} \hat{a}_{p+q}^\dagger \hat{a}_{p'-q}^\dagger \hat{a}_{p'} \hat{a}_p, \tag{3}$$

where $\varepsilon_p = p^2/2m$ and second term as $\hat{V}$. For $u = 0$ the groundstate in a grandcanonical description is a coherent state of bosons in the zero-momentum state, i.e. all particles are Bose condensed.

Finite interactions lead to scattering of bosons from the condensate into finite momentum modes and hence a depletion of the condensate fraction. However, if the interactions are weak, one can still assume that the $p = 0$ mode is macroscopically occupied, $\langle a_0^\dagger a_0 \rangle \gg 1$. As $[a_0, a_0^\dagger] = 1$, one can neglect it for a macroscopically occupied $p = 0$ mode and replace $a_0,\ a_0^\dagger$ by their expectation value $\sqrt{N_0}$, the number of bosons in the condensate. Thus our small parameter is $(N - N_0)/N_0$. One can therefore approximate all other modes to be small $a_p \ll \sqrt{N_0}$ and therefore neglect all terms in the interaction part of above Hamiltonian which contain more than two creation/annihilation operators with $p \neq 0$.

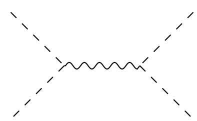

Figure 1: Interaction of condensate particles

The leading term of the expansion involves interactions solely between the stationary particles (particles of the condensate) as in fig. 1 (the dashed line corresponds to condensed particles)

$$\hat{V}_0 = \frac{\varphi}{2V} \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0.$$

There are no terms that contain only one creation or annihilation operator for non-condensate particles due to the conservation of momentum.

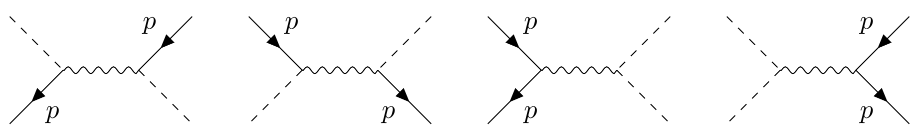

Figure 2: Interaction of condensate particle and non-condensate particle

The next four expansion terms each contain one operator of creation and one operator of annihilation above the non-condensate particles (fig. 2):

$$\hat{V}_2 = \frac{\varphi}{2V} \sum_{p \neq 0} \left(\hat{a}^\dagger \hat{a}_0 \hat{a}_0 \hat{a}_p + \hat{a}_p^\dagger \hat{a}_0^\dagger \hat{a}_p \hat{a}_0 + \hat{a}_0 \hat{a}^\dagger \hat{a}_0 \hat{a}_p + \hat{a}_p^\dagger \hat{a}_0^\dagger \hat{a}_p \hat{a}_0 \right) \stackrel{1}{=} \frac{2\varphi}{V} \hat{a}_0^\dagger \hat{a}_0 \sum_{p \neq 0} \hat{a}_p^\dagger \hat{a}_p,$$

where in $\stackrel{1}{=}$ it was used that $[\hat{a}_0, \hat{a}_p] = 0$.

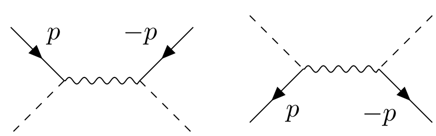

Figure 3: Creation and annihilation of two condensate particles from non-condensate

Two more terms of the expansion contain two creation operators each and two operators for annihilation condensate particles (fig. 3):

$$\hat{V}_2' = \frac{\varphi}{2V} \sum_{p \neq 0} \left(\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_p \hat{a}_{-p} + \hat{a}_p^\dagger \hat{a}_{-p}^\dagger \hat{a}_0 \hat{a}_0 \right)$$

Let's substitute into the equations $\hat{a}_0 = \hat{a}_0^\dagger = \sqrt{N_0}$ and rewrite it in terms $N = N_0 + \sum_{p \neq 0} \hat{a}_p^\dagger \hat{a}_p$. The quadratic terms in the number of non-condensate particles should be discarded. Thus, the complete Hamiltonian can be represented in the following form:

$$\hat{H} = \frac{N^2}{2V} \varphi + \sum_{p \neq 0} \epsilon_p \hat{a}_p^\dagger \hat{a}_p + \frac{N}{2V} \sum_{p \neq 0} \left(\hat{a}_p^\dagger \hat{a}_{-p}^\dagger + \hat{a}_p \hat{a}_{-p} \right), \qquad \epsilon_p = \varepsilon_p + \varphi n. \tag{4}$$

We can assume that the total number of particles is fixed and the number of condensate particles is variable, then we can work with the Hamiltonian in form (4).

2. Bogoliubov transformation. $\hat{H}$ can be diagonalized with a Bogoliubov transformation to a new set of creation and annihilation operators

$$\begin{aligned} \hat{a}_p^\dagger &= u_p \hat{\alpha}_p^\dagger + v_p \hat{\alpha}_{-p}, \\ \hat{a}_p &= u_p \hat{\alpha}_p + v_p \alpha_{-p}^\dagger. \end{aligned} \tag{5}$$

The newly introduced $\hat{\alpha}_p$ and $\hat{\alpha}_p$ have to obey bosonic commutation relations (canonical transformation):

$$[\hat{a}_p, \hat{a}_p^\dagger] = 1 = u_p^2(\hat{\alpha}_p\hat{\alpha}_p^\dagger - \hat{\alpha}_p^\dagger\hat{\alpha}_p) + v_p^2\left(\hat{\alpha}_{-p}^\dagger\hat{\alpha}_{-p} - \hat{\alpha}_{-p}\hat{\alpha}_{-p}^\dagger\right) + u_p v_p\left(\hat{\alpha}_p\hat{\alpha}_{-p} - \hat{\alpha}_{-p}\hat{\alpha}_p + \hat{\alpha}_{-p}^\dagger\hat{\alpha}_p^\dagger + \hat{\alpha}_p^\dagger\hat{\alpha}_{-p}^\dagger\right) = u_p^2 - v_p^2.$$

That allows for a convenient parametrization of the form $u_p = \cosh\theta_p$, $v_p = \sinh\theta_p$ with[1] $u, v \in \mathbb{R}$. In principle this is the same as substitution of the form $u_p = (1 - A_p^2)^{-1/2}$ and $v_P = A_p(1 - A_p^2)^{-1/2}$.

3. Diagonalization. We find the second relation after substituting (5) into the operator part of the Hamiltonian (4). Equating the coefficients in front of the products $\alpha_p^\dagger \alpha_{-p}^\dagger$ to zero, we obtain the missing equation:

$$\epsilon_p u_p v_p + \tfrac{\varphi}{2}(u_p^2 + v_p^2) = 0.$$

Now we find the unknown function A_p

$$A_p = \frac{-\epsilon_p + \sqrt{\epsilon_p^2 - (\varphi n)^2}}{\varphi n}. \tag{6}$$

Here we need to be careful with the sign. Ultimately, the Hamiltonian takes on a diagonal form

$$\hat{H} = \frac{N^2}{2V}\varphi + \sum_{p\neq 0}(\epsilon_p v_p^2 + \varphi n u_p v_p) + \sum_{p \neq 0} E_p \hat{\alpha}_p^\dagger \hat{\alpha}_p, \qquad E_p = \sqrt{\epsilon_p^2 - (\varphi n)^2} = \sqrt{\left(\frac{p^2}{2m}\right)^2 - \frac{p^2}{m}\varphi n}, \tag{7}$$

where we substitute $u_p,\ v_p$ in $E_p = \epsilon_p(u_p^2 + v_p^2) + 2\varphi n u_p v_p$. Note that the ground state $|0\rangle$ of the (7) is simply the vacuum state of Bogoliubov quasi-particles $\hat{\alpha}_p,\ \hat{\alpha}_p^\dagger$.

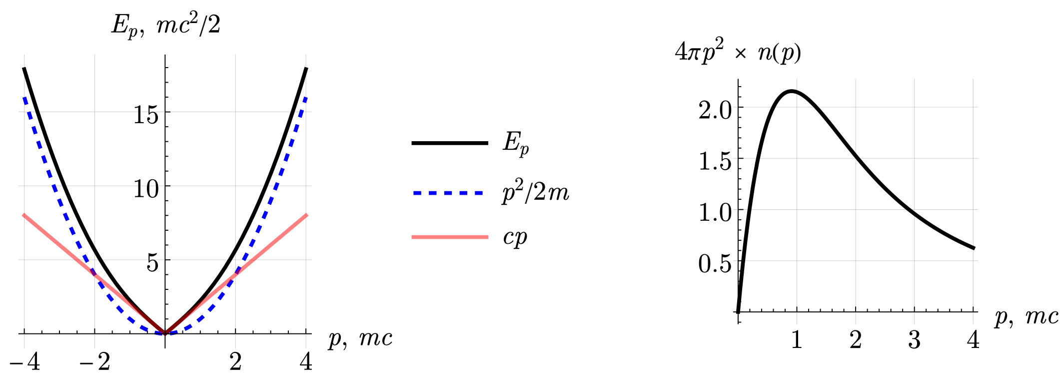

Figure 4: Exitation energy E_p and the momentum distribution function in 3D $4\pi p^2 n(p)$

4. Large canonical ensemble. In zero order ($N_0 \approx N$) we have $\hat{H} - \mu\hat{N} = -\mu N + \frac{N^2}{2V}\varphi$, thus $\Omega_0 = \langle\psi|\hat{H} - \mu\hat{N}|\psi\rangle \to \min$ and

$$\mu = \varphi n,$$

and we get $\Omega_0 = -\frac{N^2}{2V}\varphi$, so pressure is $P_0 = -\Omega_0/V$ and hydrodynamic speed of sound

$$c^2 = \frac{\partial P_0}{\partial \rho} = V\frac{\partial}{\partial(mN)}\left(-\frac{\Omega_0}{V}\right) = \frac{n\varphi}{m},$$

so we could rewrite E_p as

$$E_p = \sqrt{\left(\frac{p^2}{2m}\right)^2 + (cp)^2}, \qquad \Rightarrow \qquad E_p = \begin{cases} p^2/2m, & |p| \gg mc, \\ c|p|, & |p| \ll mc. \end{cases} \tag{8}$$

In the long-wave limit, the excitation spectrum has an acoustic character, and the calculated energy deviates from the linear law towards higher energies (fig. 4).

[1] We can do this because there are no external fields imposed on the system.

5. Ground state and compressibility. Using (7) and (6) we could calculate the ground state energy

$$\langle 0|\hat{H} - \mu\hat{N}|0\rangle = \Omega_0 = -\mu N + \frac{N^2}{2V}\varphi + \frac{1}{2}\sum_{p\neq 0}(E_p - \epsilon_p). \tag{9}$$

Yes, $\sum_{p\neq 0}(E_p - \epsilon_p)$ diverges as $E_p - \epsilon_p \approx -mn_0^2\varphi^2/p^2$ at $p \gg mc$, but for now we will ignore this and find

$$\Omega_0 = -\frac{V}{2\varphi}\mu^2 - \sum_{p>0}\left(\varepsilon_p + \mu - \sqrt{\varepsilon_p^2 - 2\varepsilon_p\mu}\right)$$

with $N = \mu V/\varphi$, $n = \mu/\varphi$. Isothermal compressibility is equal

$$\kappa = -\frac{1}{V}\frac{\partial^2\Omega}{\partial\mu^2} = \frac{1}{\varphi} + \frac{1}{V}\sum_{p>0}\frac{\sqrt{\varepsilon_p}}{(\varepsilon_p - 2\mu)^{3/2}}, \quad \Rightarrow \quad \lim_{\varphi\to 0}\kappa = +\infty,$$

corresponding to the limit of the ideal Bose gase.

6. Non-condensate particles. Now we could express explicitly the number of non-condensate particles by u-v Bogoliubov transformation $\langle\hat{a}_p^\dagger\hat{a}_p\rangle = \langle\hat{\alpha}_p^\dagger\hat{\alpha}_p\rangle + v_p^2$. Statistical distribution of elementary excitations $\langle\hat{\alpha}_p^\dagger\hat{\alpha}_p\rangle$ with $T \neq 0$ is given by the Bose distribution with $\mu = 0$

$$\langle\hat{\alpha}_p^\dagger\hat{\alpha}_p\rangle = \frac{1}{e^{\beta E_p} - 1}.$$

With $T = 0$ (fig. 4)

$$n(p) = \langle\hat{a}_p^\dagger\hat{a}_p\rangle = v_p^2 = \frac{m^2c^4}{2E_p\left(E_p + mc^2 + \frac{p^2}{2m}\right)}.$$

The total number of non-condensate particles at $T = 0$ is (3D case)

$$N - N_0 = \frac{V}{(2\pi\hbar)^3}\int_0^\infty 4\pi p^2\, dp\langle\hat{a}_p^\dagger\hat{a}_p\rangle = N\sqrt{n}\frac{(m\varphi)^{3/2}}{3\pi^2\hbar^3},$$

and corresponding «quantum depletion» of the condensate

$$\frac{N - N_0}{N} = \sqrt{n}\frac{(m\varphi)^{3/2}}{3\pi^2\hbar^3}.$$

Inserting[2] $u = \frac{4\pi a}{m}\hbar^2$, $a = 5\,\mathrm{nm}$ and $n = 10^{20}\,\mathrm{m}^{-3}$ (typical values for an ultracold atom experiment with ^{87}Rb)

$$\frac{N - N_0}{N} \approx 5\cdot 10^{-2},$$

which justifies the approximation used.

[2] I am not sure about it, but $[\varphi] = [a/m]\cdot[\hbar]^2$ according to the (3), that's why wrote φ in this way.