III. DILUTE BOSONS: BOGOLIUBOV APPROXIMATION

Markus Holzmann LPMMC, Maison de Magistère, Grenoble, and LPTMC, Jussieu, Paris markus@lptl.jussieu.fr http://www.lptl.jussieu.fr/users/markus (Dated: May 30, 2012)

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

$$|\varepsilon_1:n_1,\varepsilon_2:n_2,\ldots,\varepsilon_k:n_k,\ldots\rangle$$
 (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

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

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

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

$$a_k|\varepsilon_1:n_1,\varepsilon_2:n_2,\ldots,\varepsilon_k:n_k=1,\ldots\rangle = |\varepsilon_1:n_1,\varepsilon_2:n_2,\ldots,\varepsilon_k:n_k=0,\ldots\rangle$$
(6)

$$a_k|\varepsilon_1:n_1,\varepsilon_2:n_2,\ldots,\varepsilon_k:n_k=0,\ldots\rangle = 0$$
(7)

$$a_k^{\mathsf{T}}|\varepsilon_1:n_1,\varepsilon_2:n_2,\ldots,\varepsilon_k:n_k=0,\ldots\rangle = |\varepsilon_1:n_1,\varepsilon_2:n_2,\ldots,\varepsilon_k:n_k=1,\ldots\rangle$$
(8)

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

2

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

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

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

$$\Psi^{\dagger}(\mathbf{r}) = \sum_{k} \varphi_{k}^{*}(\mathbf{r}) a_{k}^{\dagger}$$
(13)

which satisfy

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

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

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

with

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

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

which can be written as

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

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

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

which gives

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

Note that the order of the operators is important.

B. Bose-Einstein condensation of a dilute gas: mean-field

At zero temperature, the variational principle could be applied to find the lowest energy state and we obtained the Gross-Pitaevskii equation. At finite temperature we can use a similar variational principle, namely any trial density matrix, ρ_0 , will lead to an upper bound of the free energy $F = E - TS - \mu N = -T \log Z$ of the system, at fixed chemical potential, μ .

We will write the normalized trial density matrix using a trial Hamiltonian, H_0 ,

$$\rho_0 = \frac{e^{-\beta H_0}}{Z_0} \tag{23}$$

The mean energy using this trial density matrix writes $\langle H \rangle_0$ whereas $-\langle \log \rho_0 \rangle_0$ is the entropy $(\langle \ldots \rangle_0$ denotes the quantum mechanical average using ρ_0). The free energy is then bounded by

$$F \le T \langle \log \rho_0 \rangle_0 + \langle H \rangle_0 = -T \log Z_0 + \langle H - H_0 \rangle_0 \tag{24}$$

where we can easily identify $F_0 = -T \log Z_0$ as the free energy of a system with Hamiltonian H_0 .

Thermal cloud $T > T_c$, homogeneous. Let us consider that H_0 is essentially given by the non-interacting system

$$H_0 = \sum_{\mathbf{k}} (\hbar^2 k^2 / 2m + \xi - \mu) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$$
⁽²⁵⁾

where $a_{\mathbf{k}}$ is the annihilation operator of state \mathbf{k} , and ξ is our variational paramter, a global shift of all energies, or equivalently, an effective change of the chemical potential. The corresponding free energy, F_0 , is almost the same as the ideal system calculated in the first lecture. Since

$$\langle \Psi^{\dagger}(\mathbf{r})\Psi^{\dagger}(\mathbf{r})\Psi(\mathbf{r})\Psi(\mathbf{r})\rangle_{0} = 2n(\mathbf{r}) = 2n$$
⁽²⁶⁾

we have $\langle H - H_0 \rangle_0 = \frac{Vg}{2} 2[n(\xi)]^2 - \xi V n(\xi)$, with

$$n(\xi) = g_{3/2}(e^{\beta(\mu-\xi)}) \tag{27}$$

so that we have

$$F \le \tilde{F}(\xi) \equiv F_0(\xi) + Vg[n(\xi)]^2 - \xi Vn(\xi)$$
(28)

Since

$$\frac{\partial F_0(\xi)}{\partial \xi} = -\frac{\partial F_0(\xi)}{\partial \mu} = Vn(\xi)$$
⁽²⁹⁾

we can easily minimize the right hand side of Eq. (28)

$$\frac{\partial \tilde{F}(\xi)}{\partial \xi} = Vn(\xi) + 2Vgn(\xi)n'(\xi) - Vn(\xi) - \xi Vn'(\xi) = [gn(\xi) - \xi]Vn'(\xi)$$
(30)

We see that the (true) minimum is reached for $\xi = 2gn(\xi)$. This leads to the mean-field (Hartree-Fock) equations which have to be solved self-consistently

$$n_{mf} = g_{3/2} \left(e^{\beta(\mu - 2gn_{mf})} \right)$$
(31)

since the rhs depends on n_{mf} . In the mean-field approach, Bose-Einstein condensation occurs for $\mu = 2gn_{mf}$. However, since the mean-field just leads to a shift of all energy levels, the critical density/temperature is just the same as for the ideal gas

$$n_{c,mf}\lambda^3 = 2.61...$$
 (32)

Mean-field condensed system. For a system below the Bose-Einstein transition, we have to split of the finite condensate density, n_0 . We will use n_0 as a parameter in favour of the chemical potential μ . We describe the excited state by a thermal trial density matrix with parameter ξ as above. However, since n_0 is treated as a parameter, $H - H_0$ contains all terms of H which involve n_0 . We first minimize with respect to ξ , where we get

$$\xi = 2g[n(\xi) + n_0] \tag{33}$$

Mimizining the residuals with respect to n_0 we can eliminate μ via

$$\mu = gn_0 \tag{34}$$

This constitutes a simple set of mean-field equations to describe the condensed phase.

C. 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,

$$V = \frac{g_0}{2\mathcal{V}} \sum_{\mathbf{p},\mathbf{k},\mathbf{q}} a^{\dagger}_{\mathbf{p}-\mathbf{q}} a^{\dagger}_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}} a_{\mathbf{p}}$$
(35)

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

$$V \approx \frac{g_0 N_0^2}{2\mathcal{V}} + \frac{g_0}{2\mathcal{V}} \sum_{\mathbf{k}\neq 0} \left[2a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} N_0 + a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} a_0 a_0 + a_0^{\dagger} a_0^{\dagger} a_{\mathbf{k}} a_{-\mathbf{k}} \right]$$
(36)

The total Hamiltonian then writes

$$H = \frac{g_0 N_0^2}{2\mathcal{V}} + \sum_{\mathbf{k}\neq 0} \left[\frac{k^2}{2m} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \frac{g_0}{\mathcal{V}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} N_0 \right] + \frac{g_0}{2\mathcal{V}} \sum_{\mathbf{k}\neq 0} \left[a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} a_0 a_0 + a_0^{\dagger} a_0^{\dagger} a_{\mathbf{k}} a_{-\mathbf{k}} \right]$$
(37)

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

$$a_{0}^{\dagger}a_{\mathbf{k}}N^{-1/2} = \frac{1}{\sqrt{1-A_{\mathbf{k}}^{2}}} \left(b_{\mathbf{k}} + A_{\mathbf{k}}b_{-\mathbf{k}}^{\dagger}\right)$$
(38)

$$a_{\mathbf{k}}^{\dagger} a_0 N^{-1/2} = \frac{1}{\sqrt{1 - A_{\mathbf{k}}^2}} \left(b_{\mathbf{k}}^{\dagger} + A_{\mathbf{k}} b_{-\mathbf{k}} \right)$$
(39)

We further assume that $A_{\bf k}$ depends only on $|{\bf k}|$ and is real, so that we have

$$b_{\mathbf{k}} = \frac{1}{\sqrt{N(1 - A_k^2)}} \left[a_0^{\dagger} a_{\mathbf{k}} - A_k a_{-\mathbf{k}}^{\dagger} a_0 \right]$$
(40)

and we see that the coefficient was chosen such that

$$\begin{bmatrix} b_{\mathbf{k}}, b_{\mathbf{k}}^{\dagger} \end{bmatrix} = \frac{1}{N(1 - A_{k}^{2})} \left(\begin{bmatrix} a_{0}^{\dagger}a_{k}, a_{k}^{\dagger}a_{0} \end{bmatrix} + A_{k}^{2} \begin{bmatrix} a_{-\mathbf{k}}^{\dagger}a_{0}, a_{0}^{\dagger}a_{-\mathbf{k}} \end{bmatrix} \right) = \frac{1}{N(1 - A_{k}^{2})} \left(a_{0}^{\dagger}a_{0}(1 - A_{k}^{2}) - a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + A_{k}^{2}a_{-\mathbf{k}}^{\dagger}a_{-\mathbf{k}} \right)$$

$$= 1 + \mathcal{O}(N^{-1}) = \begin{bmatrix} a_{\mathbf{k}}, a_{\mathbf{k}}^{\dagger} \end{bmatrix}$$

$$(41)$$

and all other usual commutaion relations for creation and annihilaton.

We now have

$$a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} \simeq a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}N_{0}/N = \frac{1}{1 - A_{k}^{2}} \left[b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}} + A_{k}^{2}b_{-\mathbf{k}}b_{-\mathbf{k}}^{\dagger} + A_{k}b_{-\mathbf{k}}b_{\mathbf{k}} + A_{k}b_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger} \right]$$
$$= \frac{1}{1 - A_{k}^{2}} \left[A_{k}^{2} + b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}} + A_{k}^{2}b_{-\mathbf{k}}^{\dagger}b_{-\mathbf{k}} + A_{k}b_{-\mathbf{k}}b_{\mathbf{k}} + A_{k}b_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger} \right]$$
(42)

and

$$a_{\mathbf{k}}^{\dagger}a_{-\mathbf{k}}^{\dagger}a_{0}a_{0}/N = \frac{1}{1-A_{k}^{2}} \left[A_{k}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}} + A_{k}b_{-\mathbf{k}}b_{-\mathbf{k}}^{\dagger} + b_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger} + A_{k}^{2}b_{-\mathbf{k}}b_{\mathbf{k}} \right]$$
$$= \frac{1}{1-A_{k}^{2}} \left[A_{k} + A_{k}b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}} + A_{k}b_{-\mathbf{k}}^{\dagger}b_{-\mathbf{k}} + b_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger} + A_{k}^{2}b_{-\mathbf{k}}b_{\mathbf{k}} \right]$$
(43)

The Hamiltonian now writes

$$H = \frac{g_0 N^2}{2\mathcal{V}} + \sum_{\mathbf{k}\neq 0} \frac{1}{1 - A_k^2} \left[\left(\frac{k^2}{2m} + g_0 n \right) A_k^2 + g_0 n A_k \right] + \sum_{\mathbf{k}\neq 0} \frac{1}{1 - A_k^2} \left[\left(\frac{k^2}{2m} + g_0 n \right) (1 + A_k^2) + 2g_0 n A_k \right] b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} + \sum_{\mathbf{k}\neq 0} \frac{1}{1 - A_k^2} \left[\left(\frac{k^2}{2m} + g_0 n \right) A_k + \frac{g_0 n}{2} (1 + A_k^2) \right] \left[b_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger} + b_{\mathbf{k}} b_{-\mathbf{k}} \right]$$
(44)

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

$$\left(\frac{k^2}{2m} + g_0 n\right) A_k + \frac{g_0 n}{2} (1 + A_k^2) = 0$$
(45)

$$A_k^2 + \frac{2}{g_0 n} \left[\frac{k^2}{2m} + g_0 n \right] A_k + 1 = 0$$
(46)

 or

$$A_k = \frac{1}{g_0 n} \left[-\frac{k^2}{2m} - g_0 n \pm \sqrt{\left(\frac{k^2}{2m} + g_0 n\right)^2 - (g_0 n)^2} \right]$$
(47)

$$= -x - 1 \pm \sqrt{x(x+2)}, \quad x \equiv \frac{k^2}{2mg_0 n}$$
 (48)

We then have

$$\begin{bmatrix} 1 - A_k^2 \end{bmatrix}^{-1} = \begin{bmatrix} 1 - (x+1)^2 - x(x+2) \pm 2(x+1)\sqrt{x(x+2)} \end{bmatrix}^{-1} = \begin{bmatrix} -2x(x+2) \pm 2(x+1)\sqrt{x(x+2)} \end{bmatrix}^{-1} \\ = \frac{-2x(x+2) \mp 2(x+1)\sqrt{x(x+2)}}{4x^2(x+2)^2 \mp 4(x+1)^2x(x+2)} = \frac{-2x(x+2) \mp 2(x+1)\sqrt{x(x+2)}}{4x(x+2) + [(4x^4 + 16x^3 + 16x^2) \mp (4x^4 + 16x^3 + 16x^2)]}$$
(49)

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. (48). We therefore have

$$\left[1 - A_k^2\right]^{-1} = \frac{-2x(x+2) - 2(x+1)\sqrt{x(x+2)}}{4x(x+2)} = -\frac{1}{2} - \frac{(x+1)\sqrt{x(x+2)}}{2x(x+2)}$$
(50)

Resubstituting, we get for the Hamiltonian

$$H = E_0 + \sum_{\mathbf{k}\neq 0} \omega_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$$
(51)

where E_0 is the ground state. Explicitly, we get

$$\omega_k = \sqrt{\frac{k^2}{2m} \left[\frac{k^2}{2m} + 2g_0 n\right]} \tag{52}$$

which gives a linear (sound-wave) spectrum at small k, and a free particle behavior at large momenta. Further

$$E_0/N = \frac{g_0 n}{2} - \frac{1}{2N} \sum_{\mathbf{k} \neq 0} \left[\frac{k^2}{2m} + g_0 n - \omega_k \right]$$
(53)

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

$$\omega_k = \frac{k^2}{2m} \left[1 + \frac{4mg_0 n}{k^2} \right]^{1/2} \simeq \frac{k^2}{2m} \left[1 + \frac{1}{2} \frac{4mg_0 n}{k^2} - \frac{1}{4} \left(\frac{4mg_0 n}{k^2} \right)^2 + \cdots \right] = \frac{k^2}{2m} + g_0 n - \frac{2mg_0^2 n^2}{k^2} + \cdots, \quad k \to \infty(54)$$

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

$$g_0 = \frac{g}{1 - Cak_c} \simeq g \left[1 + \frac{g}{V} \sum_{\mathbf{q} \neq 0} \frac{4m}{q^2} \right]$$
(55)

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

$$E_0/N = \frac{2\pi an}{m} \left[1 + \frac{128}{15} \sqrt{na^3/\pi} \right]$$
(56)

The non-condensed number fra of particles is given by

$$n' = \frac{1}{V} \sum_{\mathbf{k} \neq 0} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} = n \frac{8}{3} \sqrt{n a^3 / \pi}$$
(57)

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

$$n_0/n = 1 - n'/n = 1 - \frac{8}{3}\sqrt{na^3/\pi}$$
(58)

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

$$b_{\mathbf{k}}|0\rangle_{B} = 0 \tag{59}$$

Since we have

$$b_{\mathbf{k}} \sim a_0^{\dagger} a_{\mathbf{k}} - A_k a_{-\mathbf{k}}^{\dagger} a_0 \tag{60}$$

the structure of the vaccum is given by

$$|0\rangle_B \sim \left[a_0^{\dagger} a_0^{\dagger} - \sum_{\mathbf{k}\neq 0} A_k a_{-\mathbf{k}}^{\dagger} a_{\mathbf{k}}^{\dagger}\right]^{N/2} |0\rangle \tag{61}$$

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

$$\Psi_N(\mathbf{r}_1, \dots, \mathbf{r}_N) \sim \prod_{i < j} [1 + f(r_{ij})]$$
(62)

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.