Dilute Boson Gas

In this section we consider a "gas" of spinless bosons of mass m interacting through a static potential. The treatment given here is not realistic enough to quantitatively describe liquid He^4, but does capture the dramatic effect that Bose statistics has on a many particle system. The field operator has a familiar expansion,

$$\hat{\Psi}(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} a_{\vec{k}} \exp(i\vec{k} \cdot \vec{x}), \tag{1}$$

and the Hamiltonian is

$$\begin{aligned}\hat{H} &= \int d^3\vec{x}\hat{\Psi}^\dagger(\vec{x})(-\frac{\hbar^2\nabla^2}{2m})\hat{\Psi}(\vec{x}) + \frac{1}{2}\int d^3\vec{x}d^3\vec{x'}\hat{\Psi}^\dagger(\vec{x})\hat{\Psi}(\vec{x'})V(\vec{x}-\vec{x'})\hat{\Psi}(\vec{x'})\hat{\Psi}(\vec{x}). \qquad (2)\\ &= \hat{H}_0 + \hat{V}\end{aligned}$$

and the commutation relations are

$$[a_{\vec{k}}, a^\dagger_{\vec{k'}}] = \delta_{\vec{k},\vec{k'}} \tag{3}$$

Consider first the free or non-interacting ground state. Since the particles are bosons, there is nothing to prevent more than one particle being in a given state. Clearly the ground state of the free system is simply all particles at rest or having $\vec{k} = 0$. In the interacting system, there is also a *condensate*, i.e. a macroscopic number of particles with $\vec{k} = 0$. We denote the non-interacting ground state by $|\Phi^{(0)}_N>$. If we act on this state with the destruction operator for $\vec{k} = 0$, we obtain

$$a_{\vec{0}}|\Phi^{(0)}_N >= \sqrt{N}|\Phi^{(0)}_{N-1}>, \;\; a^\dagger_{\vec{0}}|\Phi^{(0)}_N >= \sqrt{N+1}|\Phi^{(0)}_{N+1}> \tag{4}$$

On the other hand, if we apply operators with $\vec{k} \neq 0$, we obtain

$$a_{\vec{k}}|\Phi^{(0)}_N >= 0, \tag{5}$$

while

$$a^\dagger_{\vec{k}}|\Phi^{(0)}_N > \tag{6}$$

is a state with

$$\hat{H}_0(a^\dagger_{\vec{k}}|\Phi^{(0)}_N >) = (\frac{\hbar^2k^2}{2m})(a^\dagger_{\vec{k}}|\Phi^{(0)}_N >) \tag{7}$$

One of the most striking features of this system is that when interactions are included, the nature of the spectrum of low-lying spectrum of states with wave vector $\vec{k}$ is completely changed. Instead of being quadratic in k as in Eq.(7), the spectrum is *linear* in k.

Wave Vector Space The first task in analyzing this system is to do all the spacial integrals in $\hat{H}_0$ and $\hat{V}$ and obtain an expression entirely in terms of creation and destruction operators. This is straightforward for $\hat{H}_0$. We have

$$\hat{H}_0 = \sum_k a^\dagger_{\vec{k}} a_{\vec{k}} (\frac{\hbar^2 k^2}{2m}). \tag{8}$$

For $\hat{V}$, we substitute a Fourier representation for each term in Eq.(2). For example, (see the Figure) we write

$$V(\vec{x} - \vec{x}') = \frac{1}{V} \sum_q \tilde{V}(\vec{q}) \exp(i\vec{q} \cdot (\vec{x} - \vec{x}')),$$

$$\hat{\Psi}(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{k_1} a_{\vec{k}_1} \exp(i\vec{k}_1 \cdot \vec{x}),$$

etc. Doing the integral $d^3\vec{x}$, we obtain

$$\int d^3\vec{x} \exp(-i\vec{k'}_1 \cdot \vec{x}) \exp(i\vec{q} \cdot (\vec{x} - \vec{x}')) \exp(i\vec{k}_1 \cdot \vec{x}) = V \delta_{-\vec{k'}_1 + \vec{q} + \vec{k}_1, 0} \exp(-i\vec{q} \cdot \vec{x}')$$

In a similar way, doing the integral $d^3\vec{x'}$, we have

$$\int d^3\vec{x'} \exp(-i\vec{k'}_2 \cdot \vec{x'}) \exp(-i\vec{q} \cdot \vec{x'}) \exp(i\vec{k}_2 \cdot \vec{x'}) = V \delta_{-\vec{k'}_2 - \vec{q} + \vec{k}_2, 0}$$

For volume factors, we have $1/V^3$ initially, and the spacial integrals produced V^2, so we have a net $1/V$. Using the Kronecker delta's to eliminate $\vec{k'}_1$ and $\vec{k'}_2$, we finally have

$$\hat{V} = \frac{1}{2V} \sum_{k_1, k_2, q} a^\dagger_{\vec{k}_1 + \vec{q}} a^\dagger_{\vec{k}_2 - \vec{q}} \tilde{V}(\vec{q}) a_{\vec{k}_2} a_{\vec{k}_1} \tag{9}$$

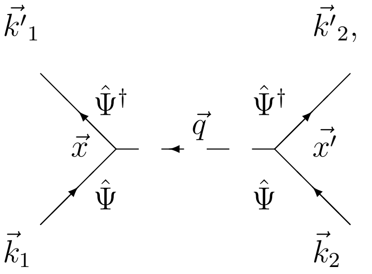
The potential is expected to be strongly repulsive at short range. We will idealize this by taking $V(\vec{x} - \vec{x'})$ to be a delta function,

$$V(\vec{x} - \vec{x'}) \equiv \lambda \delta^3(\vec{x} - \vec{x'}), \ \text{ or } \ \tilde{V}(\vec{q}) = \lambda.$$

Using this form for the potential, $\hat{V}$ becomes

$$\hat{V} = \frac{\lambda}{2V} \sum_{k_1, k_2, q} a^\dagger_{\vec{k}_1 + \vec{q}} a^\dagger_{\vec{k}_2 - \vec{q}} a_{\vec{k}_2} a_{\vec{k}_1} \tag{10}$$

Figure 1: Diagram for writing $\hat{V}$ in wave vector space



Approximating the Condensate Progress can be made in analyzing this system if it is assumed that the interacting system, like the free system, has a macroscopic number of particles in the $\vec{k}=0$ state. The Ukrainian physicist N.N. Bogoliubov then realized that it makes sense to treat $a_{\vec{0}}$ and $a^\dagger_{\vec{0}}$ as non-operators, or in Dirac's terminology, "c-numbers." For us this means that we make the replacements

$$a_{\vec{0}} \to \sqrt{N}, \;\; a^\dagger_{\vec{0}} \to \sqrt{N}. \tag{11}$$

Treated as operators, we know that

$$[a_{\vec{0}}, a^\dagger_{\vec{0}}] = 1,$$

and the replacement Eq.(11) ignores "1" compared to $\sqrt{N}$. The interacting system of course does not have literally all N particles in the condensate. We will assume that the number of particles in states with $\vec{k} \neq 0$, is a negligible fraction of the total number N, so Eq.(11) is still accurate to $O(1/N)$.

The next step in Bogoliubov's analysis is to classify terms in $\hat{V}$ in terms of the number of $a_{\vec{0}}$ and $a^\dagger_{\vec{0}}$ factors that appear, each one being replaced by $\sqrt{N}$. Doing this, it is easy to see that terms of $O((\sqrt{N})^4, (\sqrt{N})^2, (\sqrt{N})^1, 1)$ can occur, with $(\sqrt{N})^3$ ruled out because if three external lines in Fig.(1) have zero wave vector, the fourth one must as well. We write

$$\hat{V} = \hat{V}_4 + \hat{V}_2 + \hat{V}_1 + \hat{V}_0, \tag{12}$$

where $\hat{V}_j$ is proportional to $(\sqrt{N})^j$. The term $\hat{V}_4$ seems at first sight to have no operator character at all. However, some care is necessary in dealing with $\hat{V}_4$, since the number of particles must add up to N. We can certainly write

$$N = a^\dagger_0 a_0 + \sum_{k\neq 0} a^\dagger_{\vec{k}} a_{\vec{k}}, \tag{13}$$

or

$$a^\dagger_0 a_0 = N - \sum_{k\neq 0} a^\dagger_{\vec{k}} a_{\vec{k}}.$$

Now $\hat{V}_4 = \lambda a^\dagger_0 a^\dagger_0 a_0 a_0 / 2V$. Using the formula for $a^\dagger_0 a_0$, we have

$$\hat{V}_4 = \frac{\lambda}{2V}(N^2 - 2N \sum_{k\neq 0} a^\dagger_{\vec{k}} a_{\vec{k}} + O(1)). \tag{14}$$

The $O(1)$ term in $\hat{V}_4$ can be dropped in the present approximation, but the operator $O(N)$ term must be retained.

The next term to consider is $\hat{V}_2$, which has several parts. These may be understood as follows. Consider the term in $\hat{V}$ which has $\vec{k}_1 = 0$ and $\vec{k'}_1 = 0$. To be in $\hat{V}_2$, we must have $\vec{k}_2$ and $\vec{k'}_2$ non-zero. This will contribute a term to $\hat{V}_2$ equal to

$$\frac{\lambda N}{2V} \sum_{k\neq 0} a^\dagger_{\vec{k}} a_{\vec{k}}, \tag{15}$$

where we dropped the subscript on k_2. However, there is another term with $\vec{k}_1 = 0$. Instead of $\vec{k'}_1 = 0$, we may set $\vec{k'}_2 = 0$. It is easily checked that this also gives a term identical to Eq.(15). Two more terms of the same form will be generated by setting $\vec{k}_2 = 0$, and either $\vec{k'}_1 = 0$, or $\vec{k'}_2 = 0$. Altogether there are four copies of Eq.(15) in $\hat{V}_2$. There are two additional terms generated by setting either $\vec{k}_1 = 0$ and $\vec{k}_2 = 0$ or $\vec{k'}_1 = 0$ and $\vec{k'}_2 = 0$. The final form of $\hat{V}_2$ is

$$\hat{V}_2 = n\frac{\lambda}{2}\sum_k \left(4a^\dagger_{\vec{k}}a_{\vec{k}} + a^\dagger_{\vec{k}}a^\dagger_{-\vec{k}} + a_{\vec{k}}a_{-\vec{k}}\right), \tag{16}$$

where $n = N/V$ is the particle density. We may now write the Hamiltonian, keeping only operator terms, including the operator part of $\hat{V}_4$,

$$\hat{H} = \sum_k \left\{(\epsilon_{\vec{k}} + \lambda n)a^\dagger_{\vec{k}}a_{\vec{k}} + n\frac{\lambda}{2}(a^\dagger_{\vec{k}}a^\dagger_{-\vec{k}} + a_{\vec{k}}a_{-\vec{k}})\right\} + \hat{V}_1 + \hat{V}_0, \tag{17}$$

where $\epsilon_{\vec{k}} = \hbar\omega_{\vec{k}} = \hbar^2k^2/2m$. The dominant term in $\hat{H}$ is the one in $\{\cdot\}$. Although quadratic, the terms in $a^\dagger_{\vec{k}}a^\dagger_{-\vec{k}}$ and $a_{\vec{k}}a_{-\vec{k}}$ have a peculiar from and prevent any simple use of perturbation theory in the smaller terms $\hat{V}_1$ and $\hat{V}_0$. What is done next, again following Bogoliubov, is to introduce new operators to replace $a_{\vec{k}}$ and $a^\dagger_{\vec{k}}$. We define

$$a_{\vec{k}} \equiv u_{\vec{k}}b_{\vec{k}} + v_{\vec{k}}b^\dagger_{-\vec{k}} \tag{18}$$

and

$$a^\dagger_{-\vec{k}} \equiv u_{\vec{k}}b^\dagger_{-\vec{k}} + v_{\vec{k}}b_{\vec{k}},$$

where the $u_{\vec{k}}, v_{\vec{k}}$ are parameters to be determined.

Now, using the formulas Eqs.(18), we return to the Hamiltonian of Eq.(17), eliminate the a and $a^\dagger$ operators in favor of b and $b^\dagger$ operators, and choose the $u_{\vec{k}}$ and $v_{\vec{k}}$ such that there are no bb or $b^\dagger b^\dagger$ terms in the resulting Hamiltonian. The part of the resulting Hamiltonian which is quadratic in operators will then resemble a set of harmonic oscillator-type terms, summed over $\vec{k}$. This will then be the so-called "free Hamiltonian." Terms which are cubic and quartic in operators will of course remain in the full Hamiltonian. An unusual feature of the present system is that the "free Hamiltonian" contains dependence on the interaction between particle through the parameter λn.

Deriving the conditions on $u_{\vec{k}}$ and $u_{\vec{k}}$ To see what the required conditions are, first consider $a^\dagger_{\vec{k}}a_{\vec{k}}$ expressed in terms of the new operators. We have

$$a^\dagger_{\vec{k}}a_{\vec{k}} = (u_{\vec{k}}b^\dagger_{\vec{k}} + v_{\vec{k}}b_{-\vec{k}})(u_{\vec{k}}b^\dagger_{-\vec{k}} + v_{\vec{k}}b_{\vec{k}}) \tag{19}$$

$$= (u_{\vec{k}})^2(b^\dagger_{\vec{k}}b_{\vec{k}}) + (v_{\vec{k}})^2b_{-\vec{k}}b^\dagger_{-\vec{k}} + u_{\vec{k}}v_{\vec{k}}(b^\dagger_{\vec{k}}b^\dagger_{-\vec{k}} + b_{\vec{k}}b_{-\vec{k}})$$

The terms proportional to $u_{\vec{k}} v_{\vec{k}}$ are the type of terms we wish to cancel (they have either two b operators or two $b^\dagger$ operators.) Next, let us write out $a_{\vec{k}} a_{-\vec{k}}$ in terms of the new operators. We have

$$\begin{aligned} a_{\vec{k}} a_{-\vec{k}} &= (u_{\vec{k}} b_{\vec{k}} + v_{\vec{k}} b^\dagger_{-\vec{k}})(u_{\vec{k}} b_{\vec{k}} + v_{\vec{k}} b^\dagger_{-\vec{k}}) \\ &= (u_{\vec{k}})^2 b_{\vec{k}} b_{-\vec{k}} + (v_{\vec{k}})^2 b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}} + u_{\vec{k}} v_{\vec{k}} (b_{\vec{k}} b^\dagger_{\vec{k}} + b^\dagger_{-\vec{k}} b_{-\vec{k}}) \end{aligned} \tag{20}$$

In Eq.(20) the terms we wish to cancel are the coefficients of $(u_{\vec{k}})^2$ and $(v_{\vec{k}})^2$. The expansion of $a^\dagger_{\vec{k}} a^\dagger_{-\vec{k}}$ is just the adjoint of Eq.(20).

We can now find the condition we want by simply demanding that the coefficient of either $b_{\vec{k}} b_{-\vec{k}}$ or $b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}}$ vanish. Choosing $b_{\vec{k}} b_{-\vec{k}}$, we go back to the part of $\hat{H}$ inside $\{\cdot\}$ in Eq.(17) and identify $b_{\vec{k}} b_{-\vec{k}}$, terms using Eqs.(19) and (20). Setting the coefficient of these terms to zero, we have

$$(\epsilon_{\vec{k}} + \lambda n) u_{\vec{k}} v_{\vec{k}} + \frac{1}{2} \lambda n \left((u_{\vec{k}})^2 + (v_{\vec{k}})^2 \right) = 0 \tag{21}$$

It is easily checked that setting the coefficient of $b^\dagger_{\vec{k}} b^\dagger_{-\vec{k}}$ terms to zero gives the same condition as Eq.(21). Note that if we take $u_{\vec{k}} > 0$, then Eq.(21) requires that $v_{\vec{k}} < 0$. As we will see below, after solving Eq.(21) for the $u_{\vec{k}}$ and $v_{\vec{k}}$, the resulting quadratic part of the full Hamiltonian will have only $b^\dagger b$ type terms.

To solve Eq.(21), we temporarily suppress the label $\vec{k}$ and introduce the dimensionless ratio

$$s \equiv \frac{\epsilon_{\vec{k}}}{\lambda n}.$$

Rewriting Eq.(21), we have

$$(1 + s) 2uv + u^2 + v^2 = 0, \tag{22}$$

where we still have $u^2 - v^2 = 1$. Setting

$$u = \sqrt{1 + v^2},$$

we have

$$2(1 + s)(\sqrt{1 + v^2}) v + 1 + 2v^2 = 0. \tag{23}$$

Moving $1 + 2v^2$ to the right hand side and squaring the resulting equation, we have

$$4(1 + s)^2 (1 + v^2) v^2 = 1 + 4v^2 + 4v^4 \tag{24}$$

Setting

$$z = v^2,$$

Eq.(24) becomes the quadratic

$$4z^2(1 - (1 + s)^2) + 4z(1 - (1 + s)^2) + 1 = 0. \tag{25}$$

Solving Eq.(25) and restoring the $\vec{k}$ label, we have

$$(v_{\vec{k}})^2 = \frac{1}{2}\left(\frac{1+s}{\sqrt{s(2+s)}} - 1\right), \tag{26}$$

and

$$(u_{\vec{k}})^2 = 1 + (v_{\vec{k}})^2 = \frac{1}{2}\left(\frac{1+s}{\sqrt{s(2+s)}} + 1\right).$$

It is of interest to note the behavior of $(u_{\vec{k}})^2$ and $(u_{\vec{k}})^2$ for large and small values of the parameter s. For $s >> 1$, we have $\epsilon_{\vec{k}} >> \lambda n$, i.e. the kinetic energy of a freely moving particle is very large vs. λn. In this case it is easy to see that

$$(u_{\vec{k}})^2 \longrightarrow 1, \quad (v_{\vec{k}})^2 \longrightarrow 0, \tag{27}$$

or in other words the $b_{\vec{k}}$ and $b^\dagger_{\vec{k}}$ are essentially the same as the $a_{\vec{k}}$ and $a^\dagger_{\vec{k}}$. On the other hand, for $s << 1$, the factor of $1/\sqrt{s}$ in Eqs.(26) means that both $(u_{\vec{k}})^2$ and $(v_{\vec{k}})^2$ are quite large. This is the most interesting limit.

Having insured there will be no $b_{\vec{k}}b_{-\vec{k}}$ or $b^\dagger_{\vec{k}}b^\dagger_{-\vec{k}}$ in the Hamiltonian, we now return to Eqs.(17), (19) and (20) and collect the remaining terms. The $\{\cdot\}$ term in Eq.(17) is now

$$\sum_k (\epsilon_{\vec{k}} + \lambda n)\left[(u_{\vec{k}})^2 b^\dagger_{\vec{k}} b_{\vec{k}} + (v_{\vec{k}})^2 b_{-\vec{k}} b^\dagger_{-\vec{k}}\right] \tag{28}$$

$$+ \sum_k 2\lambda n u_{\vec{k}} v_{\vec{k}} \left[b_{\vec{k}} b^\dagger_{\vec{k}} + b^\dagger_{-\vec{k}} b_{-\vec{k}}\right],$$

where the factor of 2 in the second term comes from the fact that $a_{\vec{k}}a_{\vec{k}}$ and $a^\dagger_{\vec{k}}a^\dagger_{-\vec{k}}$ each contribute 2 terms so the original factor of 1/2 become a factor of 2. Substituting $\vec{k} \to -\vec{k}$, and dropping constants from $b, b^\dagger$ commutators, we finally have for the part of the Hamiltonian quadratic in b operators,

$$\sum_k b^\dagger_{\vec{k}} b_{\vec{k}} \left[((u_{\vec{k}})^2 + (v_{\vec{k}})^2)(\epsilon_{\vec{k}} + \lambda n) + 2u_{\vec{k}} v_{\vec{k}} \lambda n\right]. \tag{29}$$

The factor enclosed in $[\cdot]$ is the single particle excitation spectrum. Using Eqs.(26), we have

$$((u_{\vec{k}})^2 + (v_{\vec{k}})^2) = \frac{1+s}{\sqrt{s(1+s)}}, \quad \text{and} \quad u_{\vec{k}} v_{\vec{k}} = \frac{-1}{2\sqrt{s(1+s)}} \tag{30}$$

Using these results in Eq.(29), extracting a factor of λn, we have

$$\lambda n \sum_k b^\dagger_{\vec{k}} b_{\vec{k}} \left[(1+s)\frac{1+s}{\sqrt{s(1+s)}} - \frac{1}{\sqrt{s(1+s)}}\right] = \lambda n \sum_k b^\dagger_{\vec{k}} b_{\vec{k}} \sqrt{s(2+s)} \tag{31}$$

The single particle excitation energy is

$$\tilde{\epsilon}_{\vec{k}} = \lambda n \sqrt{s(2+s)}$$

For $s >> 1$, we have

$$\tilde{\epsilon}_{\vec{k}} \to \lambda n s = \frac{\hbar^2 k^2}{2m}$$

so in this limit, the potential between particles is ineffective and the excitation energy approaches that of free particles. However in the small s or small k limit, we have

$$\tilde{\epsilon}_{\vec{k}} \to \hbar k c_s,$$

where the "sound speed" is given by

$$c_s = \sqrt{\frac{\lambda n}{m}}.$$

Here we see that the potential between particles completely changes the spectrum, making in linear in $|\vec{k}|$ rather than quadratic. The interactions of a particle with small $|\vec{k}|$ with the condensate of $\vec{k} = 0$ particles is responsible for this difference. The linear nature of the small $|\vec{k}|$ excitations remains when the cubic and quartic terms in the Hamiltonian are considered. Bogoliubov's elegant treatment and his transformation here used in a boson system also provides a useful method in the theory of superconductivity.