Physics 127c: Statistical Mechanics

Weakly Interacting Bose Gas

Bogoliubov Theory

The Hamiltonian is

$$H = \sum_{\vec{k}} \varepsilon_k b^+_{\vec{k}} b_{\vec{k}} + \frac{1}{2\Omega} \sum_{\vec{k}\vec{k}'\vec{q}} \tilde{u}(\vec{q}) b^+_{\vec{k}+\vec{q}} b^+_{\vec{k}'-\vec{q}} b_{\vec{k}'} b_{\vec{k}}. \tag{1}$$

We will look at the weakly interacting system at low temperatures. Already, without interactions, we have Bose condensation

$$\left\langle b^+_0 b_0 \right\rangle = N_0 = N. \tag{2}$$

Interactions will reduce this, but if they are weak the *depletion of the condensate* will be a small fraction $(N - N_0)/N \ll 1$, or

$$\sum_{\vec{k}}{}' \left\langle b^+_{\vec{k}} b_{\vec{k}} \right\rangle \ll N, \tag{3}$$

with $\sum'$ denoting the sum over all $\vec{k} \neq 0$. With the macroscopic occupation of the zero mode we can neglect the quantum fluctuations relative to the mean (cf. the classical treatment of electromagnetism)

$$b_0 \to N_0^{1/2}, \quad b^+_0 \to N_0^{1/2} \tag{4}$$

where N_0 is just a number (called a *c-number* to distinguish it from an operator).

Equation (4) is now substituted into the Hamiltonian, followed by expansion in $(N - N_0)/N$. The kinetic energy term is unchanged, since there is no contribution from the $\vec{k} = 0$ state. The potential energy can be written as the sum of terms at successive order (decreasing powers of $N_0^{1/2}$) $V = V_0 + V_1 + \cdots$ with

$$V_0 = \frac{1}{2\Omega} \tilde{u}(0) N_0^2 \tag{5}$$

$$V_2 = \frac{N_0}{2\Omega} \sum_{\vec{q}}{}' \tilde{u}(\vec{q})(b^+_{\vec{q}} b^+_{-\vec{q}} + b_{\vec{q}} b_{-\vec{q}} + b^+_{-\vec{q}} b_{-\vec{q}} + b^+_{\vec{q}} b_{\vec{q}}) + \tilde{u}(0)(b^+_{\vec{q}} b_{\vec{q}} + b^+_{-\vec{q}} b_{-\vec{q}}). \tag{6}$$

(The first order term V_1 is zero by momentum conservation.) It's convenient to combine all the $\tilde{u}(0)$ terms

$$\frac{1}{2\Omega} \tilde{u}(0) N_0^2 + \frac{N_0}{2\Omega} \sum_{\vec{q}}{}' \tilde{u}(0)(b^+_{\vec{q}} b_{\vec{q}} + b^+_{-\vec{q}} b_{-\vec{q}}) \simeq \frac{1}{2\Omega} \tilde{u}(0) N^2 \tag{7}$$

leaving

$$V_2' = \frac{N_0}{2\Omega} \sum_{\vec{q}}{}' \tilde{u}(\vec{q})(b^+_{\vec{q}} b^+_{-\vec{q}} + b_{\vec{q}} b_{-\vec{q}} + b^+_{-\vec{q}} b_{-\vec{q}} + b^+_{\vec{q}} b_{\vec{q}}) \tag{8}$$

so that we can write the Hamiltonian as $H = \text{const} + H_1$ with H_1 the part to be solved

$$H_1 = \frac{1}{2} \sum_{\vec{q}}{}' [\varepsilon_q + n_0 \tilde{u}(\vec{q})](b^+_{\vec{q}} b_{\vec{q}} + b^+_{-\vec{q}} b_{-\vec{q}}) + n_0 \tilde{u}(q)(b^+_{\vec{q}} b^+_{-\vec{q}} + b_{\vec{q}} b_{-\vec{q}}) \tag{9}$$

where $n_0 = N_0/\Omega$ is the *condensate density* and since the first term in V_1' mixes $\vec{q}$ and $-\vec{q}$ we have explicitly written the kinetic energy terms from $\vec{q}$ and $-\vec{q}$.

The momentum state creation and annihilation operators $b^+_{\vec{q}}, b_{\vec{q}}$ are no longer ladder operators of the Boson Hamiltonian. We look for new creation and annihilation operators $\alpha^+_{\vec{q}}, \alpha_{\vec{q}}$ that do have this property, i.e. operators satisfying

$$[\alpha_{\vec{q}}, \alpha^+_{\vec{q}'}] = \delta_{\vec{q}\vec{q}'} \tag{10a}$$

$$[\alpha^+_{\vec{q}}, \alpha^+_{\vec{q}'}] = 0 = [\alpha_{\vec{q}}, \alpha_{\vec{q}'}] \tag{10b}$$

and in terms of which the Hamiltonian has the form

$$H_1 = \sum_{\vec{q}} E_q \alpha^+_{\vec{q}} \alpha_{\vec{q}} + \text{const}. \tag{11}$$

We look for $\alpha^+_{\vec{q}}, \alpha_{\vec{q}}$ in the form

$$\alpha_{\vec{q}} = u_q b_{\vec{q}} + v_q b^+_{-\vec{q}}, \tag{12}$$

$$\alpha^+_{\vec{q}} = u_q b^+_{\vec{q}} + v_q b_{-\vec{q}}, \tag{13}$$

with u_q, b_q depending only on $|\vec{q}|$ and real. This type of transformation, preserving the commutation rules, is called a canonical transformation. This from of the ansatz is motivated by the way $b_{\vec{q}}$ and $b^+_{-\vec{q}}$ appear in H_1. We can also argue that $\alpha^+_{\vec{q}}$ should create momentum $\hbar\vec{q}$—which a linear combination of creating at $\vec{q}$ and destroying at $-\vec{q}$ accomplishes. Note that $\alpha^+_{\vec{q}}$ no longer adds a particle to the system! This is OK because the condensate soaks up any deficit. Sorry about the notation: u_q is not related to $\tilde{u}(\vec{q})$!

We first check the commutation rules

$$[\alpha_{\vec{q}}, \alpha^+_{\vec{q}}] = u_q^2[b_{\vec{q}}, b^+_{\vec{q}}] + v_q^2[b^+_{-\vec{q}}, b_{-\vec{q}}] \tag{14a}$$

$$= u_q^2 - v_q^2. \tag{14b}$$

So we set

$$u_q^2 - v_q^2 = 1 \tag{15}$$

and can then invert Eq. (12)

$$b_{\vec{q}} = u_q \alpha_{\vec{q}} - v_q \alpha^+_{-\vec{q}}, \tag{16a}$$

$$b^+_{\vec{q}} = u_q \alpha^+_{\vec{q}} - v_q \alpha_{-\vec{q}}. \tag{16b}$$

These expressions can then be used to evaluate H_1 in terms of the α

$$\begin{aligned} H_1 = {\sum_{\vec{q}}}' &[(\varepsilon_q + n_0\tilde{u}(\vec{q}))v_q^2 - n_0\tilde{u}(\vec{q})u_q v_q] \\ &+ \frac{1}{2}{\sum_{\vec{q}}}'[(\varepsilon_q + n_0\tilde{u}(\vec{q}))(u_q^2 + v_q^2) - 2n_0\tilde{u}(\vec{q})u_q v_q](\alpha^+_{\vec{q}}\alpha_{\vec{q}} + \alpha^+_{-\vec{q}}\alpha_{-\vec{q}}) \\ &+ \frac{1}{2}{\sum_{\vec{q}}}'[-2(\varepsilon_q + n_0\tilde{u}(\vec{q}))u_q v_q + n_0\tilde{u}(\vec{q})(u_q^2 + v_q^2)](\alpha^+_{\vec{q}}\alpha^+_{-\vec{q}} + \alpha_{\vec{q}}\alpha_{-\vec{q}}). \end{aligned} \tag{17}$$

We now choose u_q, v_q to eliminate the last term

$$\frac{2u_q v_q}{u_q^2 + v_q^2} = \frac{n_0\tilde{u}(\vec{q})}{\varepsilon_q + n_0\tilde{u}(\vec{q})}. \tag{18}$$

Since $u_q^2 - v_q^2 = 1$ this is most easily solved by introducing

$$u_q = \cosh\phi_q, \quad v_q = \sinh\phi_q \tag{19}$$

and then Eq. (18) is

$$\tanh 2\phi_q = \frac{n_0\tilde{u}(\vec{q})}{\varepsilon_q + n_0\tilde{u}(\vec{q})} \tag{20}$$

and

$$u_q^2 + v_q^2 = \cosh 2\phi_q = \frac{\varepsilon_q + n_0\tilde{u}(\vec{q})}{E_q} \tag{21}$$

$$2u_q v_q = \sinh 2\phi_q = \frac{n_0\tilde{u}(\vec{q})}{E_q} \tag{22}$$

with

$$E_q = \sqrt{(\varepsilon_q + n_0\tilde{u}(\vec{q}))^2 - (n_0\tilde{u}(\vec{q}))^2} \tag{23}$$

$$= \sqrt{\frac{\hbar^2 q^2}{2m}\left(2n_0\tilde{u}(q) + \frac{\hbar^2 q^2}{2m}\right)}. \tag{24}$$

With these results H_1 can be simplified

$$H_1 = -\frac{1}{2}\sum_{\vec{q}}{}'(\varepsilon_q + n_0\tilde{u}(\vec{q}) - E_q) + \sum_{\vec{q}}{}' E_q \alpha_q^+ \alpha_q \tag{25}$$

giving the desired form. We recognize that E_q is the excitation energy spectrum of the new Bosons. Notice that E_q is linear at small q

$$E_q \simeq \sqrt{n_0\tilde{u}(0)/m}\,\hbar q \tag{26}$$

but crosses over to the free particle quadratic form for $q \gtrsim \sqrt{mn_0\tilde{u}(0)}/\hbar$. The linear spectrum at small q is crucial to the phenomenon of superfluidity.

Since $\alpha_{\vec{q}}^+, \alpha_{\vec{q}}$ are creation and annihilation operators *and* ladder operators of the Hamiltonian, we can calculate physical quantities as we did for the harmonic oscillator. For example the ground state of the interacting system $|\psi_0\rangle$ satisfies

$$\alpha_{\vec{q}}\,|\psi_0\rangle = \langle\psi_0|\,\alpha_{\vec{q}}^+ = 0 \quad \text{for all } \vec{q}. \tag{27}$$

Condensate Depletion

The condensate depletion, or the number particles excited out of the zero momentum state by the interactions in the ground state, is

$$N' = N - N_0 = \sum_{\vec{q}}{}' \left\langle \psi_0 \left| b_{\vec{q}}^+ b_{\vec{q}} \right| \psi_0 \right\rangle \tag{28}$$

$$= \sum_{\vec{q}}{}' \left\langle \psi_0 \left| (u_q\alpha_q^+ - v_q\alpha_{-q})(u_q\alpha_q - v_q\alpha_{-q}^+) \right| \psi_0 \right\rangle \tag{29}$$

$$= \sum_{\vec{q}}{}' v_q^2 = \sum_{\vec{q}}{}' \frac{1}{2}\left(\frac{\varepsilon_q + n_0\tilde{u}(\vec{q})}{E_q} - 1\right). \tag{30}$$

Since the term in () becomes unity when $E_q \simeq \varepsilon_q$, i.e. except for the small range of q (for weak interactions) where the spectrum is linear, we can replace $\tilde{u}(\vec{q})$ by $\tilde{u}(0) = g$, say. Then converting the $\vec{q}$ sum to an integral (noting that the $\vec{q} = 0$ term gives negligible contribution)

$$N' = \frac{\Omega}{(2\pi)^3} 4\pi \int_0^\infty dq\, q^2 \frac{1}{2} \left(\frac{\hbar^2 q^2/2m + n_0 g}{\sqrt{(\hbar^2 q^2/2m)(2n_0 g + \hbar^2 q^2/2m)}} - 1 \right). \tag{31}$$

Substituting $y = \sqrt{\hbar^2 q^2/2mn_0 g}$ gives

$$\frac{N'}{N_0} = \frac{1}{4\pi^2} \frac{1}{n_0} \left(\frac{2mn_0 g}{\hbar^2} \right)^{3/2} \int_0^\infty y^2 \left(\frac{y^2 + 1}{(y^4 + 2y^2)^{1/2}} - 1 \right) dy. \tag{32a}$$

The integral is $\sqrt{2}/3$, so that

$$\frac{N'}{N_0} = \frac{8}{3} \left(\frac{n_0 a^3}{\pi} \right)^{1/2} \tag{33}$$

where $a = mg/4\pi\hbar^2$ is known as the scattering length.

Note that the depletion of the condensate is small for weak interaction, g small, but the expansion in g is *nonanalytic*. This shows us that we could not get the results by simple perturbation theory: the canonical transformation goes beyond this.

Other Thermodynamic Properties

Since we have the excitation energy spectrum, and can write any physical operator in terms of the corresponding creation and annihilation operators $\alpha_{\vec{q}}^+, \alpha_{\vec{q}}$ (via their expressions in terms of $b_{\vec{q}}^+, b_{\vec{q}}$) we can now calculate the thermodynamic properties at nonzero temperature. In this, we neglect the interaction between the *new* Bosons, which would arise from the terms V_3 and V_4 containing 3 and 4 α operators. This is OK for weak interactions, except *very* near the superfluid transition temperature, where we expect the universal fluctuation behavior characteristic of superfluids. This universal behavior derives from the interactions. The linear spectrum at small q corresponds to phonon excitations (you can check that the slope is just the speed of sound in the interacting gas.) The low temperature thermodynamics will have the familiar power law behavior for these excitations, namely a T^3 specific heat. The normal fluid density will grow as T^4.

Further Reading

Now would be a good time to review Lecture 15 and problem 3 of Homework 7 for Ph127a where the physics of superfluidity was discussed. In particular, the importance of the linear spectrum $\varepsilon_k \propto k$ (rather than $\varepsilon_k \propto k^2$) and the notion of the *normal fluid density* were discussed.

Pathria §10.2-10.7 discusses the weakly interacting Bose gas.