Quantum Gases, Condensed Matter Physics 24/25

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Weakly interacting Bose gas:

Consider a system of N bosons at temperature $T = 0$ in a volume V. If the bosons are non-interacting, they are all condensed in the single-particle ground state, i.e. $|g.s.\rangle = \frac{1}{\sqrt{N!}}(a_0^\dagger)^N|0\rangle$, where $|0\rangle$ is the vacuum state. The aim of this exercise is to investigate the effect of weak interactions.

(a) Consider the Hamiltonian:

$$H = \sum_{\mathbf{k}} \epsilon_k^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2}\int d^3\mathbf{x}\, d^3\mathbf{x}' a^\dagger(\mathbf{x})a^\dagger(\mathbf{x}')U(\mathbf{x}-\mathbf{x}')a(\mathbf{x}')a(\mathbf{x}), \tag{1.1}$$

where $U(\mathbf{x}) = g\delta(\mathbf{x})$ is the interaction and $\epsilon_k^0 = \frac{k^2}{2m}$ is the single-particle kinetic energy ($\hbar = 1$). By going to Fourier space, defined by $a(\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_k e^{i\mathbf{k}\cdot\mathbf{x}}a_{\mathbf{k}}$ and $U(\mathbf{k}) = \int d^3\mathbf{x} e^{-i\mathbf{k}\cdot\mathbf{x}}U(\mathbf{x})$, show that:

$$H = \sum_{\mathbf{k}} \epsilon_k^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{g}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}/2}a^\dagger_{-\mathbf{k}+\mathbf{q}/2}a_{\mathbf{k}'+\mathbf{q}/2}a_{-\mathbf{k}'+\mathbf{q}/2}. \tag{1.2}$$

The original Hamiltonian is defined by:

$$H = \sum_k \epsilon_k^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \underbrace{+\frac{g}{2}\int_V d^3\mathbf{x}d^3\mathbf{y} a^\dagger(\mathbf{x})a^\dagger(\mathbf{y})\delta^3(\mathbf{x}-\mathbf{y})a(\mathbf{y})a(\mathbf{x})}_{\text{interaction}}$$

where $a_{\mathbf{k}}^\dagger/a_{\mathbf{k}}$ creates/anihilates a particle with momentum $\mathbf{k}$ and kinetic energy $\epsilon_k^0 = \frac{\mathbf{k}^2}{2m}$, and $a^\dagger(\mathbf{x})/a(\mathbf{x})$ does the same at position $\mathbf{x}$. So, we use $a(\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}a_{\mathbf{k}}$ to obtain:

$$\begin{aligned} H &= \sum_{\mathbf{k}} \epsilon_k^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{g}{2V^2}\sum_{\mathbf{pqrs}}\int_V d^3\mathbf{x}d^3\mathbf{y}\delta^3(\mathbf{x}-\mathbf{y})e^{-i\mathbf{p}\cdot\mathbf{x}}e^{-i\mathbf{q}\cdot\mathbf{y}}e^{i\mathbf{r}\cdot\mathbf{y}}e^{i\mathbf{s}\cdot\mathbf{x}}a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{r}}a_{\mathbf{s}} \\ &= \sum_{\mathbf{k}} \epsilon_k^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{g}{2V^2}\sum_{\mathbf{pqrs}}\underbrace{\int_V d^3\mathbf{x} e^{-i(\mathbf{p}+\mathbf{q})\cdot\mathbf{x}}e^{i(\mathbf{r}+\mathbf{s})\cdot\mathbf{x}}}_{V\delta_{\mathbf{p}+\mathbf{q}-\mathbf{r}-\mathbf{s}}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{r}}a_{\mathbf{s}}. \end{aligned}$$

And now, defining:

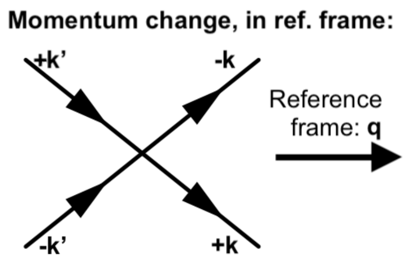
$$\mathbf{q} \equiv \mathbf{p}+\mathbf{q} = \mathbf{r}+\mathbf{s}, \quad \mathbf{k} \equiv \frac{\mathbf{p}-\mathbf{q}}{2}, \quad \mathbf{k}' = \frac{\mathbf{r}-\mathbf{s}}{2}$$

and using the delta of momentums, we get:

$$\boxed{H = \sum_{\mathbf{k}} \epsilon_k^0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{g}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}/2}a^\dagger_{-\mathbf{k}+\mathbf{q}/2}a_{\mathbf{k}'+\mathbf{q}/2}a_{-\mathbf{k}'+\mathbf{q}/2}}.$$

▷ **Interpret the momenta in the last term (a diagram would be useful).**

We can see that the last term represents an interaction between two particles, where there is an exchange of momentum $\mathbf{k}-\mathbf{k}'$ between them, but the total momentum $\mathbf{q}$ is conserved:



(b) Expand the Hamiltonian in powers of N_0, keeping for the interaction part only terms that are linear or quadratic in N_0, to find the approximate Hamiltonian:

$$H = \sum_{\mathbf{k}} \epsilon^0_k a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{g}{2V}N_0^2 + \frac{gN_0}{V}\sum_{k\neq 0}\left[a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}} + \frac{1}{2}\left(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}\right)\right]. \tag{1.3}$$

Expanding the interaction term for few excitations, neglecting terms that are not linear or quadratic in $\langle a^\dagger_0 a_0\rangle \equiv \langle N_0\rangle$, since most particles belong to the condensate, we get:

$$\begin{aligned} A \equiv & \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}/2} a^\dagger_{-\mathbf{k}+\mathbf{q}/2} a_{\mathbf{k}'+\mathbf{q}/2} a_{-\mathbf{k}'+\mathbf{q}/2} = \\ & = a^\dagger_0 a^\dagger_0 a_0 a_0 + \sum_{\mathbf{k}\neq 0}\left(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} a_0 a_0 + a^\dagger_0 a^\dagger_0 a_{\mathbf{k}} a_{-\mathbf{k}} + 4 a^\dagger_{\mathbf{k}} a^\dagger_0 a_{\mathbf{k}} a_0\right) \end{aligned}$$

which is easy to see, since we always need two terms to have 0 momenta for having at least $O({N_0}^1)$, and the remaining two will still need to conserve total momenta. Simplifying:

$$A \approx N_0^2 + N_0 \sum_{\mathbf{k}\neq 0}\left(a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + a_{\mathbf{k}} a_{-\mathbf{k}} + 4 a^\dagger_{\mathbf{k}} a_{\mathbf{k}}\right)$$

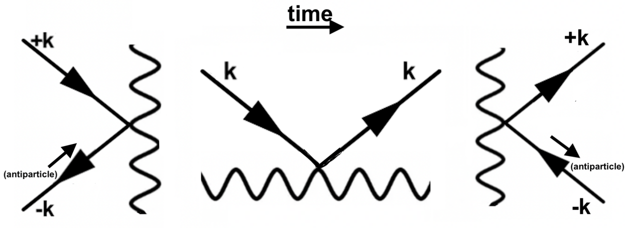
which back to the full Hamiltonian ($H = \sum_{\mathbf{k}} \epsilon^0_k a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{g}{2V}A$) gives the desired expression:

$$\boxed{H \approx \underbrace{\sum_{\mathbf{k}} \epsilon^0_k a^\dagger_{\mathbf{k}} a_{\mathbf{k}}}_{\text{Total Kinetic}} + \underbrace{\frac{g}{2V}N_0^2}_{\text{Cond. self int.}} + \frac{gN_0}{V}\sum_{\mathbf{k}\neq 0}\left[\overbrace{\underbrace{a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}}}_{N_{\mathbf{k}}+N_{-\mathbf{k}}-2N_0} + \underbrace{\frac{1}{2}(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}})}_{\text{pair prod./annih.}}}^{\text{Int. Condensate - Excitations}}\right]}.$$

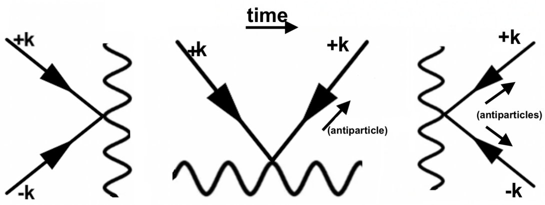
▷ **Interpret, for instance diagrammatically, the terms in the last expression.**

The first part of the last term ($N_{\mathbf{k}} + N_{-\mathbf{k}} - 2N_0$) includes interactions of the excited $(N - N_0)$ particles with the N_0 particles in the condensate, conserving the total number of excitations.

This means diagrams with two arrows, one pointing into, and the other out of the Condensate. Or what is the same, a single particle that interacts with the Condensate, or pairs of Particle-Antiparticle creation/annihilation:



The last part instead (pair prod./annih.), represents the interactions that don't conserve the total number of excitations. This means creation/annihilation of pairs of particle-particle/antip.-antip., or a particle becoming an antiparticle after interacting with the condensate:



(c) Use the relation between the total number of particles and the condensed particles $N = N_0 + \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$, to replace all N_0 in the expression, and neglect terms which have more than two creation or annihilation operators. You should find:

$$H = gn\frac{N^2}{2} + \sum_{\mathbf{k}\neq 0}\left[\left(\epsilon^0_k + gn\right)a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \frac{gn}{2}\left(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}\right)\right], \tag{1.4}$$

with $n = \frac{N}{V}$ the density.

Substituting $N_0 = N - \sum_{k\neq 0} a^\dagger_k a_k$ in the interaction, neglecting higher-orders of $O(a^2_{\mathbf{k}})$:

$$\begin{aligned} I &= \frac{g}{2V}\left(N - \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}}a_{\mathbf{k}}\right)^2 + \frac{g\left(N - \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}}a_{\mathbf{k}}\right)}{V}\sum_{\mathbf{k}\neq 0}\left[a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}} + \frac{1}{2}(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}})\right] \\ &= \frac{g}{2V}\left(N^2 - 2N\sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \cancel{O(a^4_{\mathbf{k}})}\right) + \frac{gN + \cancel{O(a^2_{\mathbf{k}})}}{V}\sum_{\mathbf{k}\neq 0}\left[a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{-\mathbf{k}}a_{-\mathbf{k}} + \frac{1}{2}(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}})\right] \end{aligned}$$

which, defining $n \equiv N/V$, makes the original Hamiltonian $H = \sum_{\mathbf{k}\neq 0} \epsilon^0_k a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + I$:

$$\boxed{H = \frac{gnN}{2} + \sum_{\mathbf{k}\neq 0}\left[(\epsilon^0_k + gn)a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \frac{gn}{2}(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}})\right]}.$$

where we see that we have effectively:

- Shifted the ground energy, to account for both Condensate and Excitations together.
- Joined the old excitations propagator and their interactions with the Condensate that conserved them, into a new effective propagator (new effective Kinetic Energy).
- Kept the interactions that didn't conserve the number of excitations, as interactions.

(d) The Bogoliubov transformation consists in defining new operators:

$$\begin{pmatrix} a_{\mathbf{k}} \\ a^{\dagger}_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \alpha_{\mathbf{k}} \\ \alpha^{\dagger}_{-\mathbf{k}} \end{pmatrix}, \tag{1.5}$$

with: $u_k = \sqrt{\frac{1}{2}\left(\frac{\epsilon_k^0+gn}{\epsilon(k)}+1\right)}$, $\quad v_k = \sqrt{\frac{1}{2}\left(\frac{\epsilon_k^0+gn}{\epsilon(k)}-1\right)}$**, so that** $u_k^2 - v_k^2 = 1$**.**
We have also introduced the Bogoliubov dispersion $\epsilon(k) = \sqrt{(\epsilon_k^0)^2 + 2gn\epsilon_k^0}$.

▷ **Show that the Bogoliubov transformation preserves the bosonic commutation relations (if you wish, do this only for** $[\alpha_k, \alpha_k^{\dagger}]$**).**

Inverting the Bogoliubov transformation we have:

$$\begin{pmatrix} \alpha_{\mathbf{k}} \\ \alpha^{\dagger}_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ a^{\dagger}_{-\mathbf{k}} \end{pmatrix} \quad \rightarrow \quad \begin{cases} \alpha_{\mathbf{k}} = u_k a_{\mathbf{k}} + v_k a^{\dagger}_{-\mathbf{k}} \\ \alpha^{\dagger}_{\mathbf{k}} = v_k a_{-\mathbf{k}} + u_k a^{\dagger}_{\mathbf{k}} \end{cases}$$

So let's jump and verify the bosonic commutation relations, with this:

$$\begin{aligned} [\alpha_k, \alpha_q^{\dagger}] &= [u_k a_{\mathbf{k}} + v_k a^{\dagger}_{-\mathbf{k}}, v_q a_{-\mathbf{q}} + u_q a^{\dagger}_{\mathbf{q}}] = [u_k a_{\mathbf{k}}, u_q a^{\dagger}_{\mathbf{k}} q] + [v_k a^{\dagger}_{-\mathbf{k}}, v_q a_{-\mathbf{q}}] \\ &= u_k u_q \underbrace{[a_{\mathbf{k}}, a^{\dagger}_{\mathbf{q}}]}_{\delta_{kq}} + v_k v_q \underbrace{[a^{\dagger}_{-\mathbf{k}}, a_{-\mathbf{q}}]}_{-\delta_{kq}} = (\underbrace{u_k u_q - v_k v_q}_{q \longleftrightarrow k})\delta_{kq} = (\underbrace{u_k^2 - v_k^2}_{1})\delta_{kq} \boxed{= \delta_{kq}} \end{aligned}$$

where in the first step, we just kept the a's and $a^{\dagger}$'s pairs, since the rest (aa or $a^{\dagger}a^{\dagger}$), are trivially zero. So the Bogoliubov transformation preserves the bosonic commutation relations.

(e) Following the Bogoliubov transformation, the Hamiltonian takes the form:

$$H = gn\frac{N}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left[\epsilon_k^0 + gn - \epsilon(k)\right] + \sum_{\mathbf{k}\neq 0} \epsilon(k)\alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}. \tag{1.6}$$

▷ **Discuss the physical meaning of the various terms.**

The first thing we notice is that the Hamiltonian is, for the first time, in Diagonal form. Meaning that we can easily extract information from its spectra, from visual inspection:

- The first two terms ($gn\frac{N^2}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}[\epsilon_k^0 + gn - \epsilon(k)]$) represent the ground state (GS) energy. We see that there is a contribution from every momentum mode $\mathbf{k}$, meaning that the GS contains excitations with every allowed momentum. Completely different from the state where every particle is in the single-particle GS.

- The last term ($\sum_{\mathbf{k}\neq 0}\epsilon(k)\alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}$) contains all the operators of the expression, and has the form of a propagator (for the Bogoliubov transformation excitations). Meaning that the Bogoliubov dispersion relation $\epsilon(k) = \sqrt{(\epsilon_k^0)^2 + 2gn\epsilon_k^0}$ gives the kinetic energy associated with an excitation $\alpha^{\dagger}_{\mathbf{k}}$.

(f) Show that the number operator $\hat{N}$ evaluated in an eigenstate of the Hamiltonian (1.6) takes the form:

$$\hat{N} = N_0 + \sum_{\mathbf{k}\neq 0} v_k^2 + \sum_{\mathbf{k}\neq 0} \left(u_k^2 + v_k^2\right) \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}}. \tag{1.7}$$

Starting from the original number operator:

$$\hat{N} = \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} = N_0 + \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} = N_0 + \sum_{k\neq 0} \left(-v_k \alpha_{-\mathbf{k}} + u_k \alpha^\dagger_{\mathbf{k}}\right)\left(u_k \alpha_{\mathbf{k}} - v_k \alpha^\dagger_{-\mathbf{k}}\right)$$

$$= N_0 + \sum_{\mathbf{k}\neq 0} \left(-u_k v_k \alpha_{-\mathbf{k}} \alpha_{\mathbf{k}} + v_k^2 \underbrace{\alpha_{-\mathbf{k}} \alpha^\dagger_{-\mathbf{k}}}_{\alpha^\dagger_{-\mathbf{k}} \alpha_{-\mathbf{k}} + 1} + u_k^2 \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} - u_k v_k \alpha^\dagger_{\mathbf{k}} \alpha^\dagger_{-\mathbf{k}} \right)$$

$$= N_0 + \sum_{\mathbf{k}\neq 0} \left[v_k^2 + (v_k^2 + u_k^2) \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} - u_k v_k \left(\alpha_{-\mathbf{k}} \alpha_{\mathbf{k}} + \alpha^\dagger_{\mathbf{k}} \alpha^\dagger_{-\mathbf{k}}\right)\right]$$

and the last term, has pairs of $\alpha_{\mathbf{k}}\alpha_{\mathbf{k}}$ & $\alpha^\dagger_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}}$ instead of $\alpha_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}}$ or $\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}}$, which don't leave the state invariant, and therefore don't contribute to the expectation value of N:

$$\boxed{\langle N \rangle = N_0 + \sum_{\mathbf{k}\neq 0} \left[v_k^2 + (v_k^2 + u_k^2) \langle \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle \right]} - \cancelto{0}{u_k v_k \langle \alpha_{-\mathbf{k}} \alpha_{\mathbf{k}} + \alpha^\dagger_{\mathbf{k}} \alpha^\dagger_{-\mathbf{k}} \rangle}$$

meaning that for an eigenstate of the Hamiltonian (1.6), we achieve the desired expression.

▷ **Discuss the meaning of the various terms.**

- The first term (N_0) is the number of particles in the single-particle ground state.
- The second term ($\sum_{\mathbf{k}\neq 0} v_k^2$) is proportional to the number of excitations with momentum $\mathbf{k}$ when the gas is in its ground state.
- The last term ($\propto \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}}$) is proportional to the number of excitations with momentum $\mathbf{k}$ above the ground state of the gas.

▷ **Show that the depletion of the condensate in the GS is:** $N - N_0 = \frac{8}{3\sqrt{\pi}} \left(na^3\right)^{1/2} N$

Let's start, from the result of the previous section:

$$N - N_0 = \sum_{k\neq 0} v_k^2 \approx \frac{V}{(2\pi\hbar)^3} \int_V v_k^2 d^3k = \frac{V}{(2\pi\hbar)^3} \int_0^\infty 4\pi k^2 v_k^2 dk$$

$$= \frac{V}{4\pi^2\hbar^3} \int_0^\infty k^2 \left(\frac{\epsilon_k^0 + gn}{\sqrt{(\epsilon_k^0)^2 + 2gn\epsilon_k^0}} - 1 \right) dk$$

and now doing a change of variable: $q = \epsilon_k^0/gn = k^2/2gnm$; $dq = kdk/2gnm$

$$N - N_0 = \frac{V}{\pi^2\hbar^3} \left(\frac{mgn}{2}\right)^{\frac{3}{2}} \underbrace{\int_0^\infty \sqrt{q} \left(\frac{q+1}{\sqrt{q(q+2)}} - 1 \right) dq}_{2\sqrt{2}/3}$$

$$= \frac{V}{3\pi^2\hbar^3} (mgn)^{\frac{3}{2}} \boxed{= \frac{8}{3\sqrt{\pi}} \sqrt{na^3} N}$$

were in the end we introduce the strength of the interaction $g = 4\pi\hbar^2 a/m$, with a being the s-wave scattering length, finally achieving the desired result.