Bose – Einstein Condensation summary

- single particle energies:

$$\varepsilon_{\vec p} = \frac{\vec p^{\,2}}{2m} = \frac{\hbar^2 \vec k^2}{2m} = \varepsilon_p$$

- mean occupation number

$$\overline{n}_p = \frac{1}{e^{\beta(\varepsilon_p - \mu)} - 1}$$

chemical potential (μ)

- total number of bosons

$$N = N_0 + \sum_{\vec p \neq 0} \overline{n}_p = N_0 + \frac{V}{(2\pi\hbar)^3} \int d^3\vec p \; \overline{n}_p$$

$$= N_0 + \frac{V}{\lambda^3} \, g_{3/2}(z)$$

N_0: number of bosons in ground state

$\sum_{\vec p \neq 0} \overline{n}_p$: bosons populating excited states

λ: thermal wave length

$$\lambda = \frac{2\pi\hbar}{\sqrt{2\pi m k_B T}}$$

z: fugacity $z = e^{\beta\mu}$

g_ν: generalised Riemann Zeta function

$$g_\nu(z) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^\nu}$$

- condensation

- below the critical temperature the chemical potential must be zero (otherwise the mean occupation number can diverge)

- at this point one has

$$\mu = 0 \rightarrow z = 1 \rightarrow g_{3/2}(1) = \underbrace{\zeta\left(\tfrac{3}{2}\right)}$$

Riemann zeta function

$$\zeta(\nu) = \sum_{l=1}^{\infty} \frac{1}{l^{\nu}}$$

- below the critical temperature one thus has

$$N = N_0 + \frac{V}{\lambda^3}\zeta\left(\tfrac{3}{2}\right) = N_0 + \frac{\lambda_c^3}{\lambda^3}\frac{V}{\lambda_c^3}\zeta\left(\tfrac{3}{2}\right)$$

$$= N_0 + \left(\frac{T}{T_c}\right)^{3/2} \underbrace{\frac{V}{\lambda_c^3}\zeta\left(\tfrac{3}{2}\right)} = N_0 + N\left(\frac{T}{T_c}\right)^{3/2}$$

at the critical point $N_0 = 0 \rightarrow \frac{V}{\lambda_c^3}\zeta\left(\tfrac{3}{2}\right) = N$

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}^{\dagger}(\vec{r}\,')\right] = \frac{1}{V} \sum_{kk'} \underbrace{\left[a_k, a^{\dagger}_{k'}\right]}_{\delta_{kk'}} e^{-i\vec{k}\cdot\vec{r} + i\vec{k}'\cdot\vec{r}\,'}$$

$$= \frac{1}{V} \sum_{k} e^{-i\vec{k}(\vec{r}-\vec{r}\,')} = \delta(\vec{r}-\vec{r}\,')$$

$$\frac{1}{V} \int d^3\vec{r}\, \frac{\hbar^2}{2m} |\vec{k}|^2 \sum_{k'k} a^{\dagger}_{k'} a_k \, e^{ir(k'-k)}$$

$$= \sum_{kk'} \frac{\hbar^2 |\vec{k}|^2}{2m} a^{\dagger}_{k'} a_k \underbrace{\frac{1}{V} \int d^3\vec{r}\, e^{ir(k'-k)}}_{\frac{1}{V} V \delta_{k'k}}$$

$$\frac{1}{V^2} \int d^3r \sum_{kk'qq'} a^{\dagger}_k a^{\dagger}_q a_{k'} a_{q'} \, e^{i\vec{r}(k+q-k'-q')}$$

$$q' = k + q - k'$$

$$H = \sum_k \varepsilon_k a_k^+ a_k + \frac{U_0}{2V}\left[N_0^2 + N_0 \sum_k \left(a_k a_{-k} + a_k^+ a_{-k}^+ + 2a_k^+ a_k + 2a_{-k}^+ a_{-k}\right)\right]$$

$$\approx \sum_k \varepsilon_k a_k^+ a_k + \frac{U_0}{2V}\Big[N^2 - N \sum_k \left(a_k^+ a_k + a_{-k}^+ a_{-k}\right)$$

$$+ N \sum_k \left(a_k a_{-k} + a_k^+ a_{-k}^+\right)$$

$$+ 2N \sum_k \left(a_k^+ a_k + a_{-k}^+ a_{-k}\right)\Big]$$

$$= \frac{1}{2} \sum_k{}' \left(\varepsilon_k + \frac{U_0 N}{2V}\right)\left(a_k^+ a_k + a_{-k}^+ a_{-k}\right)$$

$$+ \sum_k \frac{U_0 N}{2V}\left(a_k a_{-k} + a_k^+ a_{-k}^+\right) + \frac{U_0 N}{2V}$$

$$\frac{\varepsilon_1}{\varepsilon_0} = \frac{2\sinh t \cosh t}{\cosh^2 t + \sinh^2 t} = \frac{\sinh 2t}{\cosh 2t}$$

$$= \tanh 2t$$

$u^2 = \cosh^2 t$ Solve together $u^2 = 1 + v^2$

$$\frac{\varepsilon_1}{\varepsilon_0} = \frac{2uv}{u^2+v^2} = \frac{(u+v)^2 - u^2 - v^2}{u^2+v^2} = \frac{(u+v)^2}{u^2+v^2} - 1$$

$$= \frac{2uv}{1+2v^2} = \frac{2\sqrt{1+v^2}\,v}{1+2v^2} \rightarrow \left(\frac{\varepsilon_1}{\varepsilon_0}\right)^2 = \frac{4(1+v^2)v^2}{(1+2v^2)^2}$$

The weakly interacting Bose gas

- a system of noninteracting bosons undergoes at sufficiently low temperature a phase transition into a Bose-Einstein condensate

- for a homogeneous system this means that the state with zero momentum (ground state) becomes macroscopically occupied

number of bosons in zero momentum mode

$$\frac{N_0}{N} = \begin{cases} 1-\left(\frac{T}{T_c}\right)^{3/2} & ; \quad T < T_c \\ 0 & ; \quad T > T_c \end{cases}$$

total number of bosons

- the critical temperature at which this transition takes place is

volume

$$k_B T_c = \frac{2\pi}{[\zeta(\frac{3}{2})]^{2/3}} \frac{\hbar}{m\left(\frac{V}{N}\right)^{2/3}}$$

Riemann zeta function

mass of boson

- we are now interested in investigation the impact of interactions between bosons (near $T=0$)

- the Hamilton for interacting bosons is given by

$$\mathcal{H} = \int d^3\vec{r} \left[-\hat{\psi}^\dagger(\vec{r}) \frac{\hbar^2}{2m} \nabla^2 \hat{\psi}(\vec{r}) \right]$$

annihilation operator of boson at position $\vec{r}'$

$$+ \frac{1}{2} \int d^3\vec{r}\, d^3\vec{r}'\, \hat{\psi}^\dagger(\vec{r})\, \hat{\psi}^\dagger(\vec{r}')\, V(|\vec{r}-\vec{r}'|)\, \hat{\psi}(\vec{r}')\, \hat{\psi}(\vec{r})$$

interaction potential between bosons

- field operators obey

$$[\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r}')] = \delta(\vec{r}-\vec{r}')$$
$$[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')] = [\hat{\psi}^\dagger(\vec{r}), \hat{\psi}^\dagger(\vec{r}')] = 0$$

- to simplify the situation we replace the real interaction by a so-called contact interaction: $V(\vec{r}) \approx U_0\, \delta(\vec{r})$.

- this means that two particles interact only when they are at the same position, and their interaction strength is given by U_0

- note, that such approximate description is valid only at low energies (momenta) of the bosons; for high momenta a so-called regularisation is required

- using the contact interaction, the Hamiltonian becomes

$$\mathcal{H} = \int d^3\vec{r} \left[-\hat{\psi}^+(\vec{r}) \frac{\hbar^2}{2m} \nabla^2 \hat{\psi}(\vec{r}) + \frac{U_0}{2} \hat{\psi}^+(\vec{r}) \hat{\psi}^+(\vec{r}) \hat{\psi}(\vec{r}) \hat{\psi}(\vec{r}) \right]$$

- using plane waves as a basis for representing the field operators,

$$\hat{\psi}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} a_{\vec{k}} e^{-i\vec{k}\vec{r}}, \quad \hat{\psi}^+(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} a^+_{\vec{k}} e^{i\vec{k}\vec{r}},$$

where the $a_{\vec{k}}$ are bosonic operators, i.e. $[a_{\vec{k}}, a^+_{\vec{q}}] = \delta_{\vec{k}\vec{q}}$, we can write

$$\mathcal{H} = \sum_{\vec{k}} \underbrace{\frac{\hbar^2 |\vec{k}|^2}{2m}}_{\varepsilon_k} a^+_{\vec{k}} a_{\vec{k}} + \frac{U_0}{2V} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} a^+_{\vec{k}_1} a^+_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_1 + \vec{k}_2 - \vec{k}_3}$$

ε_k ... energy for creating a boson with momentum $k = |\vec{k}|$

- close to $T = 0$, which certainly is below T_c, the mode with $\vec{k} = 0$ is macroscopically occupied
- therefore we approximate the bosonic operators associated with this mode by numbers

$\hookrightarrow \quad a_0^+ \longrightarrow \sqrt{V}\,\phi_0 \quad , \quad a_0 \longrightarrow \sqrt{V}\,\phi_0^*$

- with this replacement we can write for the condensed fraction of atoms by

$$\frac{N_0}{V} = |\phi_0|^2$$

- using this approximation, and furthermore assuming that the occupation of modes with $\vec{k} \neq 0$ is small, we can also approximate,

$$\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3} a^+_{\vec{k}_1} a^+_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_1+\vec{k}_2-\vec{k}_3} \approx \overbrace{V^2 |\phi_0|^4}^{\text{zero momentum components}} +$$

$$+ V \sum_{\vec{k}}{}' \underbrace{\left[\phi_0^{*2} a_{\vec{k}} a_{-\vec{k}} + \phi_0^2 a^+_{\vec{k}} a^+_{-\vec{k}} + 2|\phi_0|^2 (a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a^+_{-\vec{k}}) \right]}$$

summation only over modes with $\vec{k} \neq 0$.

all quartic terms have been omitted, since population of these modes is assumed to be small ($\langle a^+_k a^+_p a_q a_m \rangle \ll N_0^2$)

- in the next step we make the simplifying assumption that $\phi_0 \in \mathbb{R}$ and exploit the conservation of the number of particles:

$$N = N_0 + \frac{1}{2} \sum_{\vec{k}}{}' (a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}})$$

N: total number of particles; N_0: number of particles in condensate

- using that $N \gg \langle a^+_{\vec{k}} a_{\vec{k}} \rangle$ we can approximate

$$N_0^2 = \left(N - \frac{1}{2}\sum_{\vec{k}}{}' (a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}})\right)^2$$

$$\simeq N^2 - N \sum_{\vec{k}}{}' (a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}})$$

note, that we have here replaced to operator N by a number i.e. its average value

- this allows us to eliminate

$$V|\phi_0|^2 = V\phi_0^{*2} = V\phi_0^2 = N_0$$

from the Hamiltonian, which then takes the form

$$\mathcal{H} = \frac{U_0 N^2}{2V} + \frac{1}{2}\sum_{\vec{k}}{}' \Big[(\varepsilon_k + U_0 \frac{N}{V})(a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}}) + U_0 \frac{N}{V}(a_{\vec{k}} a_{-\vec{k}} + a^+_{\vec{k}} a^+_{-\vec{k}}) \Big]$$

- note, that this Hamiltonian is only valid, when $N_0 \simeq N \gg \langle a^+_{\vec{k}} a_{\vec{k}} \rangle$

- the Hamiltonian is a quadratic form and therefore can be diagonalised analytically

- this achieved by a <u>Bogoliubov transformation</u>
- this is similar to what we did in the context of solving the quantum Ising model with a transverse field
- however, since we are here dealing with bosons, there are some differences compared to the quantum Ising model which was mapped onto fermions
- the Hamiltonian is a sum of terms of the type

$$h = \varepsilon_0 (a^+ a + b^+ b) + \varepsilon_1 (a^+ b^+ + b a)$$

- we seek new bosonic operators (α, β) which bring this Hamiltonian into a canonical form (not containing terms of the type $\alpha^+ \beta^+$)
- we make the ansatz

coefficients (assumed to be real)

$$\alpha = u a + v b^+ , \quad \beta = u b + v a^+$$

and require canonical commutation relations:

$$[\alpha, \alpha^+] = [\beta, \beta^+] = 1 , \quad [\alpha, \beta^+] = [\alpha, \beta] = 0$$

- we find

$$[\alpha, \alpha^+] = [ua + vb^+, ua^+ + vb] = u^2 \underbrace{[a, a^+]}_{=1} + v^2 \underbrace{[b^+, b]}_{=-1} \overset{!}{=} 1$$

- hence, the coefficients u and v have to obey $u^2 - v^2 = 1$
- note, that this is different compared to fermions, where we found a relative '+' sign
- the inverse transformation is

$$a = u\alpha - v\beta^+ , \quad b = u\beta - v\alpha^+$$

and inserting it into the Hamiltonian h, yields

$$h = 2v^2\varepsilon_0 - 2uv\varepsilon_1 + [\varepsilon_0(u^2+v^2) - 2uv\varepsilon_1](\alpha^+\alpha + \beta^+\beta)$$

$$+ \underbrace{[\varepsilon_1(u^2+v^2) - 2uv\varepsilon_0]}_{\text{we require this to be zero}}(\alpha\beta + \alpha^+\beta^+)$$

- parameterising $u = \cosh t$, $v = \sinh t$, which automatically imposes $u^2 - v^2 = 1$, we find

$$\varepsilon_1(u^2+v^2) - 2uv\varepsilon_0 = \varepsilon_1(\cosh^2 t + \sinh^2 t) - 2\varepsilon_0 \sinh t \cosh t = 0$$

- This yields $\tanh 2t = \frac{\varepsilon_1}{\varepsilon_0}$ and leads to

$$u^2 = \frac{1}{2}\left(\frac{\varepsilon_0}{\varepsilon} + 1\right) \quad \text{and} \quad v^2 = \frac{1}{2}\left(\frac{\varepsilon_0}{\varepsilon} - 1\right)$$

with $\varepsilon = \sqrt{\varepsilon_0^2 - \varepsilon_1^2}$

- This leads to the diagonalised form of the Hamiltonian:

$$h = \varepsilon(\alpha^+\alpha + \beta^+\beta) + \varepsilon - \varepsilon_0$$

- applying these results to the BEC Hamiltonian yields

$$a_{\vec{k}} = u_{\vec{k}}\,\alpha_{\vec{k}} - v_{\vec{k}}\,\alpha^+_{-\vec{k}}, \quad a_{-\vec{k}} = u_{-\vec{k}}\,\alpha_{-\vec{k}} - v_{\vec{k}}\,\alpha^+_{\vec{k}}$$

$$\hookrightarrow \mathcal{H} = \frac{U_0 N^2}{2V} - \frac{1}{2}\sum_{\vec{k}}{}'\left(\varepsilon_k + U_0\frac{N}{V} - E_k\right) + \frac{1}{2}\sum_{\vec{k}}{}' E_k\left(\alpha^+_{\vec{k}}\alpha_{\vec{k}} + \alpha^+_{-\vec{k}}\alpha_{-\vec{k}}\right)$$

with $E_k = \sqrt{\varepsilon_k\left(\varepsilon_k + 2U_0\frac{N}{V}\right)}$ } excitation spectrum of the BEC

and
$$u^2_{\vec{k}} = u_k^2 = \frac{1}{2}\left[\frac{\varepsilon_k + U_0\frac{N}{V}}{E_k} + 1\right]$$

$$v^2_{\vec{k}} = v_k^2 = \frac{1}{2}\left[\frac{\varepsilon_k + U_0\frac{N}{V}}{E_k} - 1\right]$$

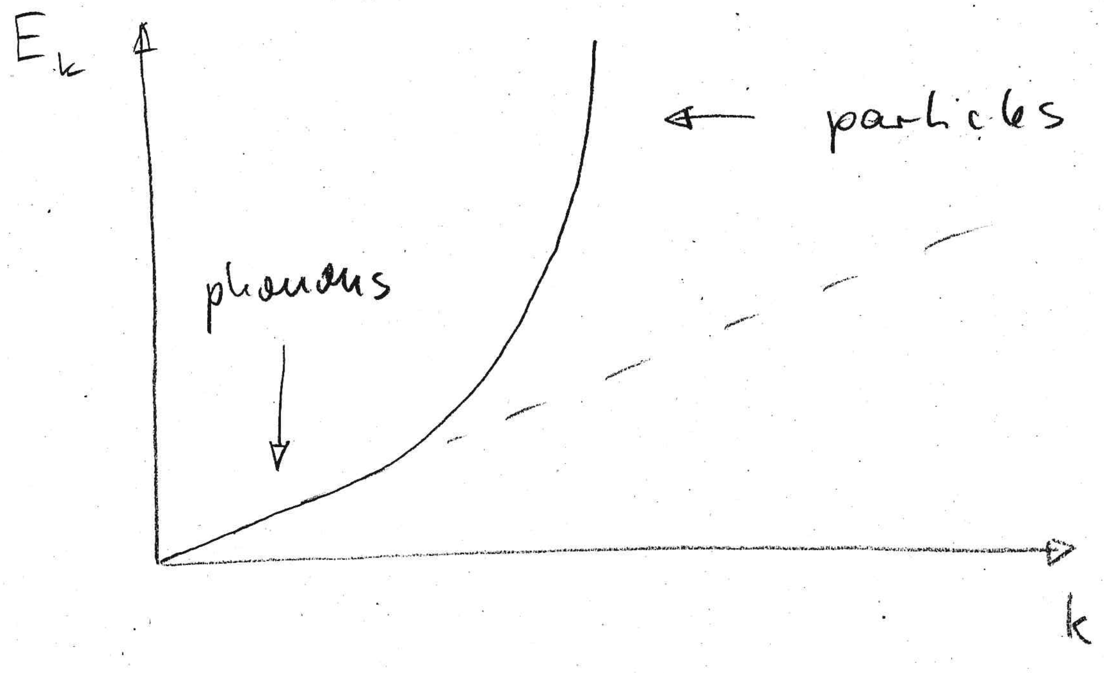
- This result shows, that for small wave vectors, where $\varepsilon_k \ll 2U_0 \frac{N}{V}$, the dispersion relation is approximately linear

  $\hookrightarrow$ $E_k \approx \hbar c |k|$ where $c = \sqrt{\frac{U_0 N}{mV}}$

  can be interpreted as the sound velocity of the elementary (quasi-particle) excitations, which are phonons

- Conversely, when $\varepsilon_k \gg 2U_0 \frac{N}{V}$ the dispersion relation becomes

  $E_k \approx \frac{\hbar^2 k^2}{2m}$ and the elementary excitations are particles with mass m



- with these results one can show that interactions actually reduce the number of particles in the condensate, which is referred to as <u>condensate depletion</u>

- to see this we express the particle number in terms of the quasi particle creation and annihilation operators

$$N = N_0 + \sum_{\vec{k}}{}' v_k^2 + \sum_{\vec{k}}{}' (u_k^2 + v_k^2)\,\alpha^+_{\vec{k}}\alpha_{\vec{k}} - \sum_{\vec{k}}{}' u_k v_k \left(\alpha^+_{\vec{k}}\alpha^+_{-\vec{k}} + \alpha_{-\vec{k}}\alpha_{\vec{k}}\right)$$

- at zero temperature no quasi-particles will be excited and the BEC is in its ground state: $|0\rangle$ with $\alpha_k|0\rangle = 0$

- hence, $\underbrace{\langle N\rangle - N_0}_{\text{number of particles not in the ground state}} = \langle 0|N|0\rangle - N_0 = \sum_{\vec{k}}{}' v_k^2$

$$= V\int \frac{d^3\vec{k}}{(2\pi)^3}\, v_k^2 = \frac{V}{(2\pi)^3}\, 4\pi \int_0^\infty dk\, k^2\, v_k^2$$

$$= \frac{V}{2\pi^2}\int_0^\infty dk\, k^2 \left(\frac{\frac{\hbar^2 k^2}{2m} + u_0\frac{N}{V}}{\left[\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2u_0\frac{N}{V}\right)\right]^{1/2}} - 1 \right)$$

$$= \frac{V}{2\pi^2} \int_0^\infty dk\, k^2 \frac{k^2+\gamma}{\sqrt{k^2(k^2+2\gamma)}} = \frac{V}{6\pi^2} \sqrt{2}\, \gamma^{3/2}$$

with $\gamma = \frac{2m U_0}{\hbar^2} \frac{N}{V}$

$$\hookrightarrow \underbrace{\frac{\langle N \rangle - N_0}{N}}_{\substack{\text{fraction of} \\ \text{atoms outside} \\ \text{the condensate}}} = \frac{N - N_0}{N} = \frac{1}{3\pi} \sqrt{\frac{m^3 U_0^3}{\hbar^3} \frac{N}{V}}$$

- finally, we consider the ground state energy of the condensate and how it is changed by interactions
- this can in principle be calculated via

$$E_0 = \langle 0 | \mathcal{H} | 0 \rangle = \frac{U_0 N^2}{2V} - \frac{1}{2} \sum_{\vec{k}}{}' \left(\varepsilon_k + U_0 \frac{N}{V} - E_k \right)$$

- however, the sum over the momenta is divergent, which stems from the fact that the contact interaction, as we used it, is incorrect for high momenta

- when treating the contact interaction in a way that is consistent also for high momenta, one obtains

$$E_0 = \frac{U_0 N^2}{2V} - \frac{1}{2}\sum_{\vec{k}}\left[\varepsilon_k + U_0\frac{N}{V} - E_k \underbrace{- \frac{1}{2\varepsilon_k}\left(\frac{U_0 N}{V}\right)^2}_{}\right]$$

term, which regularises divergence of the sum

- converting the sum to an integral then leads to the following expression for the energy density of the ground state:

$$\frac{E_0}{V} = \frac{U_0 N^2}{2V^2} + \frac{8}{15\pi^2}\left(\frac{\sqrt{m}}{\hbar}\right)^3\left(U_0\frac{N}{V}\right)^{5/2}$$