

§ 3. Bosons

*) Bose-Einstein condensation (BEC)

$$\hat{H} = \int d^d\vec{r} \hat{\psi}^+(\vec{r}) \left(-\frac{\nabla^2}{2m} - \mu \right) \hat{\psi}(\vec{r}) + \frac{1}{2} \int d^d\vec{r} d^d\vec{r}' \hat{\psi}^+(\vec{r}) \hat{\psi}^+(\vec{r}') V(\vec{r}-\vec{r}') \underbrace{\hat{\psi}(\vec{r}') \hat{\psi}(\vec{r})}_{\text{short-range interactions}}$$

partition function:

$$Z = \text{Tr } e^{-\beta \hat{H}} = \int D\bar{\psi} D\psi e^{-S[\bar{\psi}, \psi]} \quad \bar{\psi}, \psi : \text{ complex variables}$$

$$S[\bar{\psi}, \psi] = S_{\text{Berry}} + \int_0^\beta d\tau \underbrace{\hat{H}(\tau)}_{\substack{\uparrow \\ \text{normal-ordered!}}} \quad \begin{aligned} \text{S}[\bar{\psi}, \psi] &= S_{\text{Berry}} + \int_0^\beta d\tau \hat{H}(\tau) \\ &\uparrow \end{aligned}$$

Consider δ -potential for simplicity:

$$V(\vec{r}-\vec{r}') = g \delta^d(\vec{r}-\vec{r}') \quad g > 0 \quad (\text{repulsive interaction})$$

$$\Rightarrow S[\bar{\psi}, \psi] = \int_0^\beta d\tau \int d^d\vec{r} \left[\bar{\psi}(\vec{r}, \tau) \left(\partial_\tau - \frac{\nabla^2}{2m} - \mu \right) \psi(\vec{r}, \tau) + \frac{1}{2} g \underbrace{\bar{\psi}(\vec{r}, \tau) \bar{\psi}(\vec{r}, \tau) \psi(\vec{r}, \tau) \psi(\vec{r}, \tau)}_{\parallel} \right]$$

$$\left[\bar{\psi}(\vec{r}, \tau) \psi(\vec{r}, \tau) \right]^2$$

- Non-interacting case : $g = 0$

$$S_0 = \int_0^T d\tau \int d^d\vec{r} \underbrace{\bar{\psi}(\vec{r}, \tau)}_{\text{underbrace}} (\partial_\tau - \frac{\nabla^2}{2m} - \mu) \underbrace{\psi(\vec{r}, \tau)}_{\text{underbrace}}$$

$$\left\{ \begin{array}{l} \psi(\vec{r}, \tau) = \frac{1}{\sqrt{\beta V}} \sum_{\vec{k}, i\omega_n} a(\vec{k}, i\omega_n) e^{i\vec{k} \cdot \vec{r} - i\omega_n \tau} \\ \bar{\psi}(\vec{r}, \tau) = \frac{1}{\sqrt{\beta V}} \sum_{\vec{k}, i\omega_n} \bar{a}(\vec{k}, i\omega_n) e^{-i\vec{k} \cdot \vec{r} - i\omega_n \tau} \end{array} \right.$$

$$= \sum_{\vec{k}, i\omega_n} \left(-i\omega_n + \frac{|\vec{k}|^2}{2m} - \mu \right) \bar{a}(\vec{k}, i\omega_n) a(\vec{k}, i\omega_n)$$

V: volume of the system

$$\left\{ \begin{array}{l} \text{Particle number } N \\ \text{Particle density } \rho = \frac{N}{V} \end{array} \right.$$

$$\left\{ \begin{array}{l} \frac{1}{V} \int_0^T d\tau e^{i(\omega_n - \omega_{n'})\tau} = \delta_{\omega_n, \omega_{n'}} \\ \frac{1}{V} \int d^d\vec{r} e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} = \delta_{\vec{k}, \vec{k}'} \end{array} \right.$$

$$N = \int d^d\vec{r} \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle_T$$

→ determine chemical potential

- Thermal Green's function (useful tool for many-body calculations)

$$G(\vec{r}, \tau; \vec{r}', \tau') \equiv - \langle T_\tau \underbrace{\hat{\psi}(\vec{r}, \tau) \hat{\psi}^\dagger(\vec{r}', \tau')}_{\text{time-ordering}} \rangle$$

operators in Heisenberg picture

$$= \begin{cases} - \langle \hat{\psi}(\vec{r}, \tau) \hat{\psi}^\dagger(\vec{r}', \tau') \rangle & \text{for } \tau > \tau' \\ - \langle \hat{\psi}^\dagger(\vec{r}', \tau') \hat{\psi}(\vec{r}, \tau) \rangle & \text{for } \tau < \tau' \end{cases}$$

Operators in Heisenberg picture (imaginary-time evolution):

$$\hat{A}(\tau) = e^{\tau \hat{H}} \underbrace{\hat{A}(0)}_{\hat{A}} e^{-\tau \hat{H}} \quad (\text{c.f. QM-1.pdf and use } \tau = it)$$

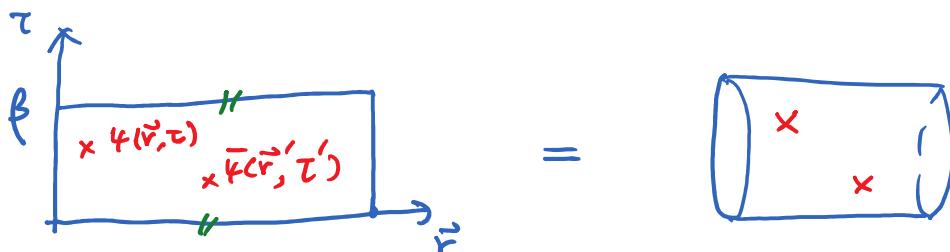
\hat{A} : operator in Schrödinger's picture

For $\tau > \tau'$:

$$\begin{aligned} G(\vec{r}, \tau; \vec{r}', \tau') &= - \langle \hat{q}(\vec{r}, \tau) \hat{q}^+(\vec{r}', \tau') \rangle_T \\ &= -\frac{1}{Z} \text{Tr} [e^{-\beta \hat{H}} \hat{q}(\vec{r}, \tau) \hat{q}^+(\vec{r}', \tau')] \\ &= -\frac{1}{Z} \text{Tr} [\underbrace{e^{-\beta \hat{H}}}_{\text{Called "trace" part below}} \underbrace{e^{\tau \hat{H}}}_{\text{evolution time}} \hat{q}(\vec{r}, 0) \underbrace{e^{-\tau \hat{H}}}_{\beta - \tau > 0} \underbrace{e^{\tau' \hat{H}}}_{\tau - \tau' > 0} \hat{q}^+(\vec{r}', 0) \underbrace{e^{-\tau' \hat{H}}}_{\tau' > 0}] \\ &= -\frac{1}{Z} \text{Tr} [\underbrace{e^{-(\beta - \tau) \hat{H}}}_{\text{evolution time}} \hat{q}(\vec{r}, 0) \underbrace{e^{-(\tau - \tau') \hat{H}}}_{\tau - \tau' > 0} \hat{q}^+(\vec{r}', 0) \underbrace{e^{-\tau' \hat{H}}}_{\tau' > 0}] \end{aligned}$$

(Similar expression can be obtained when $\tau < \tau'$.)

Space-time path integral picture for the "trace" part:



You may derive a path-integral form for the "trace" part, which is very similar to the derivation for $Z = \text{Tr} e^{-\beta \hat{H}}$ but with extra operators inserted (at given time and position)

path integral formulation :

$$G(\vec{r}, \tau; \vec{r}', \tau') = \frac{1}{Z} \int D\bar{\psi} D\psi \underbrace{[-i\bar{\psi}(\vec{r}, \tau)\bar{\psi}(\vec{r}', \tau')]}_{-\bar{\psi}\psi} e^{-S[\bar{\psi}, \psi]}$$

- 1) Generally true, not restricted to non-interacting case
- 2) Automatically time-ordered in path integral formulation
(check this from the infinite time-slice derivation)

Non-interacting case ($g=0$, $S=S_0$) :

$$\begin{aligned} G(\vec{r}, \tau; \vec{r}', \tau') &= \frac{1}{Z} \int D\bar{\psi} D\psi \underbrace{[-i\bar{\psi}(\vec{r}, \tau)\bar{\psi}(\vec{r}', \tau')]}_{-\bar{\psi}\psi} e^{-S_0[\bar{\psi}, \psi]} \\ &= \frac{-1}{\beta V} \sum_{\vec{k}_1, i\omega_1} \sum_{\vec{k}_2, i\omega_2} \frac{1}{Z} \int D\bar{a} Da \underbrace{a(\vec{k}_1, i\omega_1) \bar{a}(\vec{k}_2, i\omega_2)}_{\bar{a}a} e^{-S_0[\bar{a}, a]} \\ &\quad \times e^{i\vec{k}_1 \cdot \vec{r} - i\omega_1 \tau} e^{-i\vec{k}_2 \cdot \vec{r}' + i\omega_2 \tau'} \end{aligned}$$

Fourier transformation

Gaussian integral can be worked out as follows:

$$\left\{ \begin{array}{l} \bar{a}(\vec{k}, i\omega) = a'(\vec{k}, i\omega) - i a''(\vec{k}, i\omega) \\ a(\vec{k}, i\omega) = a'(\vec{k}, i\omega) + i a''(\vec{k}, i\omega) \end{array} \right.$$

a' and a'' real

(5)

$$\begin{aligned}
 & \frac{1}{Z} \int D\bar{a} D a \, a(\vec{k}_1, i\omega_1) \bar{a}(\vec{k}_2, i\omega_2) e^{\sum_{\vec{k}, i\omega} (i\omega - \frac{|\vec{k}|^2}{2m} + \mu) \bar{a}(\vec{k}, i\omega) a(\vec{k}, i\omega)} \\
 &= \frac{1}{Z} \int \prod_{\vec{k}, i\omega} da'(\vec{k}, i\omega) da''(\vec{k}, i\omega) \xrightarrow{\text{constant from the Jacobian}} \text{should be canceled from} \\
 & \quad \text{the same constant in } Z! \\
 & \quad \times \left(\underbrace{a'(\vec{k}_1, i\omega_1) + i a''(\vec{k}_1, i\omega_1)}_{\text{green}} \right) \left(\underbrace{a'(\vec{k}_2, i\omega_2) - i a''(\vec{k}_2, i\omega_2)}_{\text{red}} \right) \\
 & \quad \times e^{\sum_{\vec{k}, i\omega} (i\omega - \frac{|\vec{k}|^2}{2m} + \mu) [a'(\vec{k}, i\omega)^2 + a''(\vec{k}, i\omega)^2]} \\
 &= \frac{1}{Z} \int \prod_{\vec{k}, i\omega} da' da'' \\
 & \quad \times \left[a'(\vec{k}_1, i\omega_1)^2 + a''(\vec{k}_1, i\omega_1)^2 \right] \delta_{\vec{k}_1, \vec{k}_2} \delta_{\omega_1, \omega_2} \xrightarrow{\int_{-\infty}^{\infty} x e^{-\alpha x^2} = 0} \int_{-\infty}^{\infty} x^2 e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \cdot \frac{1}{2\alpha} \\
 & \quad \times e^{\sum_{\vec{k}, i\omega} (i\omega - \frac{|\vec{k}|^2}{2m} + \mu) [a'(\vec{k}, i\omega)^2 + a''(\vec{k}, i\omega)^2]} \\
 &= 2 \cdot \frac{1}{2 \left[-\left(i\omega_1 - \frac{|\vec{k}_1|^2}{2m} + \mu \right) \right]} \delta_{\vec{k}_1, \vec{k}_2} \delta_{\omega_1, \omega_2} \\
 &= \frac{-1}{i\omega_1 - \frac{|\vec{k}_1|^2}{2m} + \mu} \delta_{\vec{k}_1, \vec{k}_2} \delta_{\omega_1, \omega_2}
 \end{aligned}$$

Substitute this back to $G(\vec{r}, \tau; \vec{r}', \tau')$:

$$G(\vec{r}, \tau; \vec{r}', \tau') = \frac{1}{\beta V} \sum_{\vec{k}_1, i\omega_1} \frac{1}{i\omega_1 - \frac{|\vec{k}_1|^2}{2m} + \mu} e^{i\vec{k}_1 \cdot (\vec{r} - \vec{r}') - i\omega_1(\tau - \tau')} \underset{G(\vec{k}_1, i\omega_1)}{=} G(\vec{k}_1, i\omega_1)$$

The above form can be viewed as the Fourier transformation of the thermal Green's function.

Similarly,

$$\begin{aligned} G(\vec{k}, \tau; \vec{k}', \tau') &= -\langle T_\tau \hat{a}_{\vec{k}}(\tau) \hat{a}_{\vec{k}'}^+(\tau') \rangle \\ &= \frac{1}{\beta} \sum_{i\omega_n} \frac{1}{i\omega_n - \frac{|\vec{k}|^2}{2m} + \mu} e^{-i\omega_n(\tau - \tau')} \delta_{\vec{k}, \vec{k}'} \end{aligned}$$

Now we can use these results:

$$\begin{aligned} N &= \int d^d \vec{r} \langle \hat{\psi}^+(\vec{r}) \hat{\psi}(\vec{r}) \rangle_T \\ &= \sum_{\vec{k}} \langle \hat{a}_{\vec{k}}^+ \hat{a}_{\vec{k}} \rangle \\ &= \sum_{\vec{k}} \lim_{\tau \rightarrow 0^-} \underbrace{\langle T_\tau \hat{a}_{\vec{k}}(\tau) \hat{a}_{\vec{k}}^+(0) \rangle}_{\text{||}} \\ &\quad - G(\vec{k}, \tau; \vec{k}, 0) \\ &= - \sum_{\vec{k}} \lim_{\tau \rightarrow 0^-} \underbrace{\frac{1}{\beta} \sum_{i\omega_n} \frac{1}{i\omega_n - \frac{|\vec{k}|^2}{2m} + \mu} e^{-i\omega_n \tau}}_{\text{||}} \end{aligned}$$



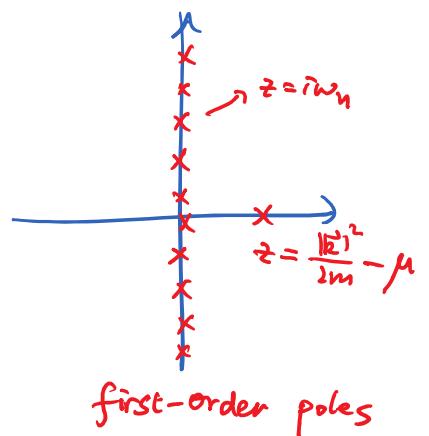
Summation over bosonic Matsubara frequency

$$\frac{1}{\beta} \sum_{i\omega_n} \frac{1}{i\omega_n - \frac{|\vec{k}|^2}{2m} + \mu} e^{-i\omega_n 0^-}$$

Introduce auxiliary function:

$$0 = \oint_C \frac{dz}{2\pi i} \underbrace{\frac{1}{e^{\beta z} - 1}}_{n_B(z)} \frac{1}{z - \frac{|\vec{k}|^2}{2m} + \mu} e^{-z\tau} \xrightarrow{z \rightarrow 0^-} (e^{-z \cdot 0^-} \text{ ensures convergence})$$

$$\Rightarrow \frac{1}{\beta} \sum_{i\vec{n}} \frac{1}{i\omega_n - \frac{|\vec{k}|^2}{2m} + \mu} e^{-i\omega_n \tau} + \frac{1}{e^{\beta(\frac{|\vec{k}|^2}{2m} - \mu)} - 1} = 0$$



(see also Wikipedia page "Matsubara frequency", where there is a table of Matsubara frequency summations.)

Substitute this into the expression for N in previous page.

$$N = - \sum_{\vec{k}} \frac{-1}{e^{\beta(\frac{|\vec{k}|^2}{2m} - \mu)} - 1}$$

$$= \sum_{\vec{k}} n_B\left(\frac{|\vec{k}|^2}{2m} - \mu\right)$$

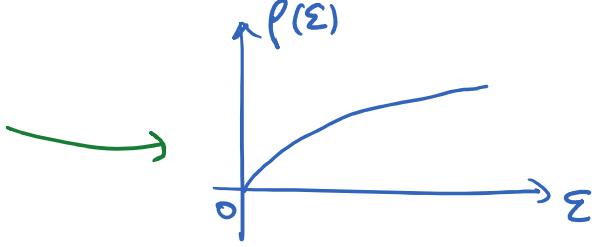
This is certainly what we would expect from the Hamiltonian formulation.

$$\hat{H} = \sum_{\vec{k}} \left(\frac{|\vec{k}|^2}{2m} - \mu\right) \hat{a}_{\vec{k}}^\dagger \hat{a}_{\vec{k}}$$

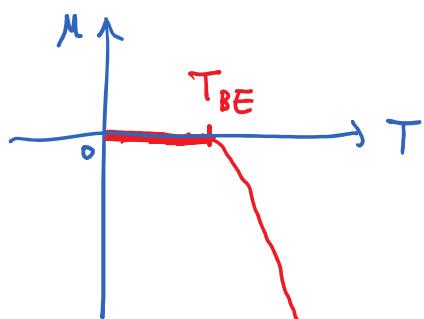
This is the starting point for analyzing whether BEC occurs. The situation gets complicated when one needs to consider dimensionality, finite/infinite system, absence/existence of trap, ...

Standard textbook example: $d=3$ Bose gas

The \vec{k} -summation/integration can be worked out by introducing density-of-states.

$$\begin{aligned}
 \rho(\varepsilon) &= \frac{1}{V} \sum_{\vec{k}} \delta\left(\varepsilon - \frac{|\vec{k}|^2}{2m}\right) \\
 &= \int \frac{d^3 k}{(2\pi)^3} \delta\left(\varepsilon - \frac{|\vec{k}|^2}{2m}\right) \\
 &= \frac{1}{(2\pi)^3} \int_0^\infty dk \ 4\pi k^2 \underbrace{\delta\left(\varepsilon - \frac{k^2}{2m}\right)}_{\sqrt{\frac{m}{2\varepsilon}} \left[\delta(k + \sqrt{2m\varepsilon}) + \delta(k - \sqrt{2m\varepsilon}) \right]} \\
 &= \frac{1}{2\pi^2} \cdot 2m\varepsilon \sqrt{\frac{m}{2\varepsilon}} \\
 &= \frac{1}{\sqrt{2\pi^2}} m^{3/2} \sqrt{\varepsilon}
 \end{aligned}$$


$$\begin{aligned}
 \Rightarrow N &= \sum_{\vec{k}} \frac{1}{e^{\beta(\frac{|\vec{k}|^2}{2m} - \mu)} - 1} \\
 &= \int_0^\infty d\varepsilon \underbrace{\sum_{\vec{k}} \delta\left(\varepsilon - \frac{|\vec{k}|^2}{2m}\right)}_{\sqrt{V\rho(\varepsilon)}} \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \\
 &= \frac{V}{\sqrt{2\pi^2}} m^{3/2} \int_0^\infty d\varepsilon \frac{\sqrt{\varepsilon}}{e^{\beta(\varepsilon - \mu)} - 1}
 \end{aligned}$$



T_{BE} : transition temperature

Bose-Einstein condensation

$$T_{BE} \approx 3.31 \left(\frac{N}{V} \right)^{2/3} \frac{\hbar^2}{m} \quad (\hbar \text{ restored})$$

Further analysis can be found in standard statistical physics books.

Go back to the path integral formulation:

$$S_0 = \sum_{\vec{k}, i\omega_n} \left(-i\omega_n + \frac{|\vec{k}|^2}{2m} - \mu \right) \bar{a}(\vec{k}, i\omega_n) a(\vec{k}, i\omega_n)$$

$$\vec{k}=0, i\omega_n=0 \text{ component: } S_0[\bar{a}_0, a_0] = -\mu |a_0|^2$$

When $\mu=0$ (BEC occurs), $|a_0|^2$ macroscopically large!

$$T=0 : \hat{H} = \sum_{\vec{k}} \left(\frac{|\vec{k}|^2}{2m} - \mu \right) \underbrace{\hat{a}_{\vec{k}}^\dagger \hat{a}_{\vec{k}}} \equiv 0$$

$$\text{Ground state } |\Psi_0\rangle = \frac{1}{\sqrt{N!}} \underbrace{(\hat{a}_{\vec{k}=0}^\dagger)^N}_{\downarrow} |0\rangle$$

All bosons are in $\vec{k}=0$ state.

$0 < T < T_{BE}$: condensate fraction $|a_0|^2 \sim N$

non-condensate fraction $\underbrace{N - |a_0|^2}_{\text{thermally activated occupied states } (|\vec{k}| \neq 0)}$