Bose-Einstein condensation and its real-space implications

one-body density matrix (OBDM)

$$g^{(1)}(\vec{r}, \vec{r}\,') = \langle \hat{\psi}^+(\vec{r})\, \hat{\psi}(\vec{r}\,') \rangle$$

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

in a translationally invariant system

$$g^{(1)}(\vec{r}, \vec{r}\,') = g^{(1)}(\vec{r}-\vec{r}\,') = \frac{1}{V} \sum_{\vec{k}} e^{-i\vec{k}(\vec{r}-\vec{r}\,')} \cdot \langle \hat{n}_{\vec{k}} \rangle$$

$$\langle \hat{n}_{\vec{k}} \rangle = \langle \hat{a}^+_{\vec{k}} \hat{a}_{\vec{k}} \rangle$$

in an ideal Bose gas in free space

BEC phase : $\quad g^{(1)}(\vec{r}, \vec{r}\,') \xrightarrow[|\vec{r}-\vec{r}\,'| \to \infty]{} \text{const.} = n_0 = \frac{N_0}{V}$

$N_0 = \langle \hat{n}_{k=0} \rangle \sim O(N)$ $\longleftrightarrow$ long-ranged correlations

$n_0(n) = O\left(\frac{N}{V}\right)$

Generalize this picture $\rightarrow$ interacting bosons

equivalent in extended systems $\quad \langle n_{k=0} \rangle = N_0 \sim O(N) \iff g^{(1)}(\vec{r}, \vec{r}\,') \xrightarrow[|\vec{r}-\vec{r}\,'| \to \infty]{} \text{const}$

input $\quad \left(g^{(1)}(\vec{r}_i, \vec{r}\,'_j)\right)^* = g^*_{ij} = \langle \hat{\psi}^+(\vec{r}) \hat{\psi}(\vec{r}\,') \rangle^*$

$$= \langle \psi^+(\vec{r}\,') \psi(\vec{r}) \rangle = g^{(1)}(\vec{r}\,', \vec{r}) = g_{ji}$$

g_{ij} is hermitian

"eigenfunctions" of $g^{(1)}$: natural orbitals

$\chi_\alpha(\vec{r})$:

$$\int d^d r' \, g^{(1)}(\vec{r}\,', \vec{r}) \, \chi_\alpha(\vec{r}\,') = \lambda_\alpha \, \chi_\alpha(\vec{r})$$

$\rightarrow$ $\underline{\underline{\chi_\alpha(\vec{r})}}$ orthonormal eigenfunctions basis for $L^2(\mathbb{R}^d)$

$\lambda_\alpha \in \mathbb{R}$

$\downarrow$

(for transl. invariant systems : $\chi_\alpha(\vec{r}) \rightarrow \dfrac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}$)

$$\Rightarrow \hat{\psi}(\vec{r}) = \sum_\alpha \chi_\alpha(\vec{r}) \, \hat{a}_\alpha \quad \Leftarrow$$

$$g^{(1)}(\vec{r}, \vec{r}\,') = \sum_{\alpha\beta} \chi^*_\alpha(\vec{r}) \, \chi_\beta(\vec{r}\,') \, \langle \hat{a}^\dagger_\alpha \hat{a}_\beta \rangle$$

$\Downarrow$

$\delta_{\alpha\beta} \langle \hat{a}^\dagger_\alpha \hat{a}_\alpha \rangle$

$(\hat{n}_\alpha)$

$v^{(j)*}_\alpha$ $\quad v^{(i)}_\alpha$ $\quad \lambda_\alpha \geq 0$

$$= \sum_\alpha \chi^*_\alpha(\vec{r}_j) \, \chi_\alpha(\vec{r}\,'_i) \, \langle \hat{n}_\alpha \rangle$$

spectral decomposition

($A \vec{v}_\alpha = \lambda_\alpha \vec{v}_\alpha$

$$A = \sum_\alpha \lambda_\alpha \, \vec{v}_\alpha \, \vec{v}_\alpha^{\,\dagger}$$

$$A_{ij} = \sum_\alpha \lambda_\alpha \, v^{(i)}_\alpha \, v^{(j)*}_\alpha$$)

In a translationally invariant system:

$$g^{(1)}(\vec r, \vec r\,') = \sum_{\vec k} \underbrace{\frac{e^{-i\vec k\cdot\vec r}}{\sqrt V}}_{\chi^*_\alpha(\vec r)} \underbrace{\frac{e^{i\vec k\cdot\vec r\,'}}{\sqrt V}}_{\chi_\alpha(\vec r\,')} \underbrace{\langle \hat n_{\vec k}\rangle}_{\lambda_\alpha}$$

<u>General definition of **BEC**</u> (Penrose - Onsager 1956)

in the spectrum of OBDM $\{\lambda_\alpha\}$

$$\exists\ \lambda_0 = \langle n_{\alpha=0}\rangle = N_0 \sim O(N)$$

$\longrightarrow$ $\chi_0(\vec r)$ lowest natural orbital

single-particle state that hosts a macroscopic fraction of the particles

$$\hat H = \sum_i \hat H_i + \hat V$$

Off-diagonal long-range order & spontaneous symmetry breaking

$$g^{(1)}(\vec r, \vec r') = \sum_\alpha \lambda_\alpha \chi^*_\alpha(\vec r)\, \chi_\alpha(\vec r')$$

BEC

$$= \underbrace{N_0\, \chi^*_0(\vec r)\, \chi_0(\vec r')}_{\sim O(N)} + \sum_{\alpha\neq 0} \lambda_\alpha \chi^*_\alpha(\vec r)\, \chi_\alpha(\vec r')$$

$\lambda_{\alpha\neq 0} \sim O(1)$

$$\chi_\alpha(\vec r) = |\chi_\alpha(\vec r)|\, e^{i\phi_\alpha(\vec r)}$$

$$\underset{|\vec r - \vec r'| \to \infty}{=} N_0\, \chi^*_0(\vec r)\, \chi_0(\vec r') + \sum_{\alpha\neq 0} \lambda_\alpha\, |\chi_\alpha(\vec r)|\, |\chi_\alpha(\vec r')|\, e^{i(\phi_\alpha(\vec r) - \phi_\alpha(\vec r'))}$$

$O(1)$ $\quad O\left(\frac{1}{V}\right)$

$\sim O(N - N_0)$

$\sim O(N)$

$\{\alpha = \vec k$

$\vec k \cdot (\vec r - \vec r')$

extended system

$\chi_0(\vec r)$ does not vanish at long distances

(α)

- volume V

$$\chi_\alpha \sim O\left(\frac{1}{\sqrt V}\right)$$

$|\vec r - \vec r'| \to \infty$

sum of $O(N)$ randomly fluctuating complex numbers of order $O\left(\frac{1}{V}\right) \sim O\left(\frac{\sqrt N}{\sqrt V \sqrt V}\right)$

(w_α is a random number $\in [-1, 1]$ $\quad \sum_{\alpha=1}^{N} w_\alpha \sim O(\sqrt N)$) $\quad \sim O\left(\frac{\sqrt N}{\sqrt V}\right)$

$$\xrightarrow{|\vec r - \vec r\,'| \to \infty} \underbrace{N_0 \uparrow \underbrace{\chi_0^*(\vec r)\,\chi_0(\vec r\,')}_{o\left(\frac{1}{V}\right)}}_{o(n)} + o\left(\frac{1}{\sqrt{V}}\right)$$

Thermodynamic limit: $N, V \to \infty$

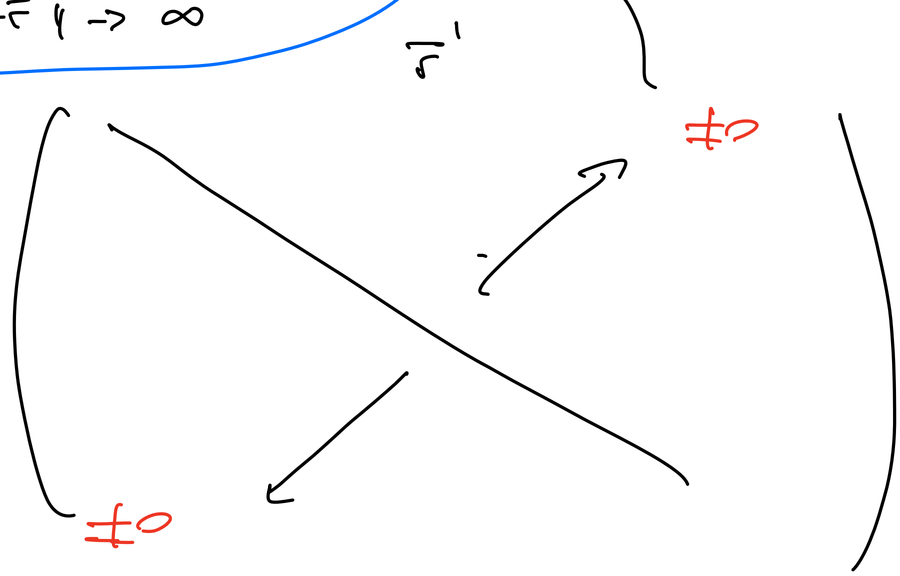
$\frac{N}{V} = n =$ const.

transl. inv. system $\qquad \chi_0(\vec r) = \frac{1}{\sqrt{V}} = \left.\frac{e^{i\vec k\cdot\vec r}}{\sqrt{V}}\right|_{\vec k = 0}$

$$g^{(1)}(\vec r, \vec r\,') \longrightarrow \frac{N_0}{V} = n_0$$

$$g^{(1)}(\vec r, \vec r\,') \longrightarrow \text{const.} \neq 0$$
$$|\vec r - \vec r\,'| \to \infty$$

$g^{(1)} =$ $\vec r$



off-diagonal long-range order

(ODLRO)

Magnets : long-range order (ferromagnetism
anti ferromagnetism
...)

$\vec{S}_i$ $\vec{S}_j$

$\uparrow \quad \uparrow \quad \hat{\imath} \quad - - - \cdot \hat{\imath}$

$g^{(1)} = \langle \hat{\psi}^{+}(\vec{r}) \, \hat{\psi}(\vec{r}\,') \rangle \xrightarrow[\text{magnets}]{} \langle \vec{S}_i \cdot \vec{S}_j \rangle$

spin-spin
correlation function

SSB

$|\vec{r}-\vec{r}\,'| \to \infty$

$\langle \hat{\psi}^{+}(\vec{r}) \rangle \langle \hat{\psi}(\vec{r}\,') \rangle$

SSB

$\xrightarrow[|i-j| \to \infty]{} \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle$

$\langle \vec{S}_i \rangle \neq 0$

conclusion : ODLRO

$\Rightarrow \langle \hat{\psi}(\vec{r}) \rangle \neq 0$

Considerations:

1) SSB $\to$ $\langle \hat{\psi}(\vec{r}) \rangle \neq 0$ as for magnets

2) physically you should cautious

implications of $\langle \hat{\psi} \rangle \neq 0$

$\uparrow$

ground state $|\Phi_0\rangle$ $\qquad \underbrace{\langle \Phi_0 | \hat{\psi}(\vec{r}) | \Phi_0 \rangle}$ $\neq 0$

$\Longleftrightarrow$ $|\Phi_0\rangle$ does not have a well-defined particle number.

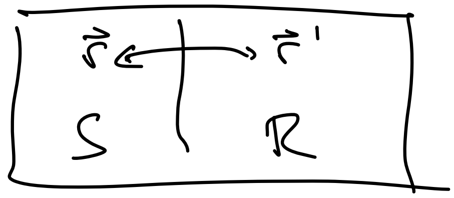
mathematically <u>plausible</u> $\quad |\Phi_0\rangle = \sum_N c_N \, |\chi_0^{(N)}\rangle$

SSB

$$\boxed{\text{ODLRO} \Longleftrightarrow \langle \psi(\vec r) \rangle \neq 0}$$

not a physical result

but a mathematical <u>trick</u>



system $\qquad$ reservoir

$$\langle \hat\psi^\dagger(\vec r)\, \hat\psi(\vec r\,') \rangle \neq 0$$

$$\langle \hat\psi(\vec r) \rangle = 0$$

symmetry that is broken: particle number conservation

$$\hat N = \int d^3r \; \psi^\dagger(\vec r)\, \psi(\vec r)$$

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

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

$$[\hat{\mathcal H} - \mu \hat N \,,\, \hat N] = 0$$

$$e^{i\phi \hat N}\, \hat{\mathcal H}\, e^{-i\phi \hat N} = \hat{\mathcal H} \qquad \phi \in \mathbb R$$

rotation $e^{i\phi\hat{N}}\,\hat{\psi}\,e^{-i\phi\hat{N}} = e^{-i\phi}\,\hat{\psi}$ (ex.)

$\langle\hat{\psi}\rangle \neq 0$

$H = \sum_{ij} J_{ij}\,\vec{S}_i\cdot\vec{S}_j$ but $\vec{S}_i$ is not rotationally invariant

In the following: use $\langle\hat{\psi}\rangle \neq 0$ as a tool for calculations (but don't believe it!) "convenient fiction"

Theory of the weakly interacting Bose gas in the presence of condensation ($\Rightarrow$ SSB)

$$g^{(1)}(\vec{r},\vec{r}\,') \xrightarrow[|\vec{r}-\vec{r}\,'|\to\infty]{} N_0\,\chi_0^*(\vec{r})\,\chi_0(\vec{r}\,') + O\left(\frac{1}{\sqrt{V}}\right)$$

$$\stackrel{SSB}{=} \langle\psi^\dagger(\vec{r})\rangle\,\langle\psi(\vec{r}\,')\rangle$$

macroscopic wavefunction (order parameter)

analog of $\langle \vec{S}_i \rangle$

$$\Psi_0(\vec{r}) = \sqrt{N_0}\; \chi_0(\vec{r})$$

$$\int d^d r \; |\Psi_0(\vec{r})|^2 = N_0 \sim O(N)$$

$\longrightarrow$ SSB $\quad \langle \hat{\psi}(\vec{r}) \rangle = \Psi_0(\vec{r})$

similar to $m = \langle \vec{S}_i \rangle$ for a ferromagnet

$\chi_\alpha(\vec{r})$ is an orthonormal basis

$$\hat{\psi}(\vec{r}) = \sum_\alpha \chi_\alpha(\vec{r})\, \hat{a}_\alpha$$

$$= \chi_0(\vec{r})\, \hat{a}_0 + \sum_{\alpha \neq 0} \chi_\alpha(\vec{r})\, \hat{a}_\alpha$$

if I am interested in states such that

$$N_0 = \langle \hat{a}_0^\dagger \hat{a}_0 \rangle \underset{N\to\infty}{\sim} O(N)$$

$$\left\langle \frac{\hat{a}_0^\dagger}{\sqrt{N}} \frac{\hat{a}_0}{\sqrt{N}} \right\rangle \underset{N\to\infty}{\sim} O(1)$$

$$\Rightarrow \left[\frac{\hat{a}_0}{\sqrt{N}}, \frac{\hat{a}_0^\dagger}{\sqrt{N}} \right] = \frac{1}{N} \xrightarrow[N\to\infty]{} 0$$

$\frac{\hat{a}_0}{\sqrt{N}}, \frac{\hat{a}_0^\dagger}{\sqrt{N}} \xrightarrow[N\to\infty]{}$ can be treated mathematically as numbers !

$\longrightarrow \quad \hat{a}_0, \quad \hat{a}_0^\dagger \quad \xrightarrow[N\to\infty]{} \quad \sqrt{N_0}\, e^{i\phi}, \quad \sqrt{N_0}\, e^{-i\phi}$ $\quad \phi = 0$

particle-num. conservation is broken

Bogolyubov replacement (shift)

$$\hat{\psi}(\vec{r}) \cong \underbrace{\sqrt{N_0}\,\chi_0(\vec{r})}_{\Phi_0(\vec{r})} + \underbrace{\sum_{\alpha\neq 0} \chi_\alpha(\vec{r})\,\hat{a}_\alpha}_{\delta\hat{\psi}}$$

scalar ?

$$= \Phi_0(\vec{r}) + \delta\hat{\psi}(\vec{r})$$

$$\langle \hat{\psi}(\vec{r}) \rangle = \Phi_0(\vec{r}) \qquad \langle \delta\hat{\psi} \rangle = 0$$

condensate

$$\underset{N}{\langle \hat{N} \rangle} = \int d^d r \, \langle \hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r}) \rangle = \int d^d r \left(\overset{N_0}{|\Phi_0|^2} + \Phi_0^* \overset{0}{\cancel{\langle \delta\psi \rangle}} + \text{c.c.} + \underline{\langle \delta\psi^\dagger \delta\psi \rangle} \right)$$

$$= N_0 + \underbrace{\int d^d r \, \langle \delta\hat{\psi}^\dagger \, \delta\hat{\psi} \rangle}_{N - N_0}$$

Non-interacting Bose gas @ $T=0$

$\underline{N_0 = N}$ $\qquad \delta\psi, \ \delta\psi^\dagger$: I can ignore them

Weakly interacting Bose gas

working assumption : $N - N_0 \neq 0$

$N - N_0 \ll N,\ N_0$

$\langle \delta\psi^\dagger \delta\psi \rangle$ is small compared to $n_0 = \frac{N_0}{V}$

density of non-condensed particle

$\downarrow$

(condensate depletion)

$\delta\psi$ is "small" compared to Ψ_0

$$\hat{\psi}(\vec{r}) = \Psi_0(\vec{r}) + \underline{\delta\hat{\psi}}(\vec{r})$$

$$\hat{H} - \mu\hat{N} = \int d^3r \; \psi^\dagger(\vec{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ext}(\vec{r}) - \mu \right] \psi(\vec{r})$$

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

$$\hat{H} - \mu\hat{N} = E_{GP}[\Psi_0, \Psi_0^*] + \hat{H}_1 + \hat{H}_2 + \hat{H}_3 + \hat{H}_4$$

Gross-Pitaevskii functional

$$E_{GP}[\Psi_0, \Psi_0^*]$$

$$= \int d^d r \, \Psi_0^*(\vec{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + U_{ext}(\vec{r}) - \mu \right] \Psi_0(\vec{r})$$

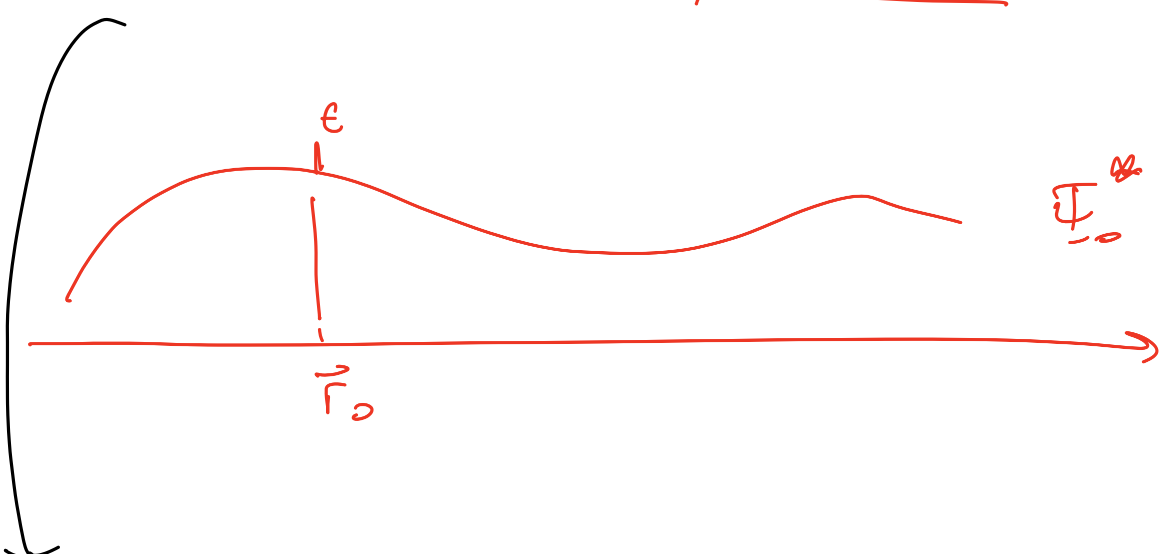
$$+ \frac{1}{2} \int d^d r \, d^d r' \, V(\vec{r} - \vec{r}') \underbrace{|\Psi_0(\vec{r})|^2}_{\Psi_0^* \Psi_0} \underbrace{|\Psi_0(\vec{r}')|^2}_{\Psi_0^* \Psi_0}$$

to find the g.s.: find the minimum of E_{GP} functional

$$\frac{\delta E_{GP}}{\delta \Psi_0^*(\vec{r}_0)} = 0 \qquad \forall \vec{r}_0$$

$$E_{GP}[\Psi_0, \Psi_0^*] = \int d^d r \, f(\Psi_0(\vec{r}) \Psi_0^*(\vec{r}))$$

$$E_{GP}[\Psi_0, \Psi_0^*(\vec{r}) + \epsilon \, \delta(\vec{r} - \vec{r}_0)]$$



$$= \int d^d r \; \underbrace{f\left(\Psi_0(\vec{r}), \; \Psi_0^*(\vec{r}) + \epsilon\, \delta(\vec{r}-\vec{r}_0) \right)}$$

$$= E_{GP}[\Psi_0, \Psi_0^*] + \epsilon \underbrace{\int d^d r \, \frac{\partial f}{\partial \Psi_0^*(\vec{r})} \delta(\vec{r}-\vec{r}_0)}$$

$$\underbrace{\left. \frac{\partial f}{\partial \Psi_0^*(\vec{r})} \right|_{\vec{r}=\vec{r}_0}}$$

$$= \frac{\delta E_{GP}}{\delta \Psi_0^*(\vec{r}_0)}$$

$$\frac{\delta E_{GP}}{\delta \Psi_0^*(\vec{r})} = 0 \qquad \forall \vec{r}$$

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + U_{ext}(\vec{r}) + \int d^d r' \, V(\vec{r}-\vec{r}\,') |\Psi_0(\vec{r}\,')|^2 \right] \Psi_0(\vec{r})$$

$$= \mu \, \Psi_0(\vec{r})$$

time-independ. Gross-Pitaevskii equation (GPE)

$\Rightarrow$ non-linear Schrödinger's equation

time - dependent GPE

$$\boxed{\hat{\psi}(\vec{r}) \to \Psi_0(\vec{r})}$$

$\uparrow$

Heisenberg equation

$$i\hbar \frac{\partial \hat{\psi}(\vec{r},t)}{\partial t} = \underbrace{\left[\hat{\psi}(\vec{r},t), \hat{H}\right]}$$

$$= \left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ext}(\vec{r},t) + \int d^d r' \, V(\vec{r}-\vec{r}\,')\, \hat{\psi}^\dagger(\vec{r}\,',t)\, \hat{\psi}(\vec{r}\,',t)\right] \hat{\psi}(\vec{r},t)$$

$$i\hbar \frac{\partial \Psi_0(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ext}(\vec{r},t) + \int d^d r' \, V(\vec{r}-\vec{r}\,') \left|\Psi_0(\vec{r}\,',t)\right|^2\right] \Psi_0(\vec{r},t)$$