Steklov Mathematical Institute of RAS, Moscow

New Trends in Mathematical Physics

Novembre 7 - 11, 2022

Why do bosons condense ?

Valentin A. ZAGREBNOV

Institut de Mathématiques de Marseille - Université d'Aix-Marseille

• *Conventional* Bose-Einstein Condensation (BEC) of the Perfact Bose-Gas: Einstein (1925), Uhlenbeck (1927), F.London (1938),... **experiments** (^4He, 1974), $n_0(T = 1,2K) = 3,4\%$...
• *Generalised* BEC *à la van den Berg-Lewis-Pulé*: Casimir (1968), van den Berg-Lewis-Pulé (1978),... **experiments** (BEC in "cigar" **traps**, 2000-2003) Beau-Zagrebnov (2010), $\boldsymbol{\lambda}_{\mathbf{T}} = \sqrt{2\pi\hbar^2/m\,\theta}$ ...
• *Non-conventional* condensate: Huang-Yang-Luttinger model (1957-1988), Bogoliubov-WIBG model (1947-1998), Zagrebnov-Bru (1998-2008), ... **experiments** (^4He pairs, 2020), Zagrebnov (2021), ...

1.0 Perfect Bose-Gas: A.Einstein (1925),G.Uhlenbeck (1927), F.London (1938), H.Casimir (1968), van den Berg-Lewis-Pulé (1978), ... Lewis-Pulé-Zagrebnov (1986), ...

• For $\Lambda = L_1 \times L_2 \times L_3 \in \mathbb{R}^3$, $\{L_j := V^{\alpha_j}\}_{j=1}^3$, $V := |\Lambda|$, the *one-particle* self-adjoint Hamiltonian $t_\Lambda := (-\Delta/2)_{p.b.}$ for periodic boundary (p.b.) conditions with Dom$(t_\Lambda) \subset L^2(\Lambda)$ and spectrum:

$$\sigma(t_\Lambda) = \{\varepsilon_k = \frac{1}{2}\sum_{j=1}^{3} k_j^2\}_{k\in\Lambda^*}, \ \Lambda^* := \{k_j = \frac{2\pi s_j}{V^{\alpha_j}}, \ s_j \in \mathbb{Z}\}_{j=1}^3.$$

• One-particle eigenfunctions: $\psi_k(x) = e^{i\,k\cdot x}/\sqrt{V}$, $k \in \Lambda^*$, $x \in \Lambda$.

• Eigenfunctions of $N = \sum_{k\in\Lambda^*} N_k$ **bosons** in the box Λ are *symmetrised* tensor products $(\otimes_{k\in\Lambda^*}\psi_k)_{symm}(X_N) = \Psi_{\{N_k\}_{k\in\Lambda^*}}(X_N)$.

• This one-to-one correspondence between *eigenfunctions* and *occupation* numbers $\{N_k \geq 0\}_{k\in\Lambda^*}$ allows explicit analysis of many *non-interacting* bosons with energy spectrum $\sum_{k\in\Lambda^*} \varepsilon_k N_k$.

• Gibbs grand-canonical ensemble (β, μ): Perfect Bose-Gas

(a) *Independent* **random variables** $k \mapsto N_k \in \mathbb{N} \cup \{0\}$, $k \in \Lambda^*$, on the probability space $\Omega := \times_{k \in \Lambda^*} \Omega_k$ of configurations $\{N_k\}_{k \in \Lambda^*}$.

(b) For *bosons* the one-mode random *occupation* numbers are: $N_k \geq 0$ for **temperature** $\theta := \beta^{-1} > 0$ and **chemical potential** $\mu \in \mathbb{R}$ (for *fermions*: $(\otimes_{k \in \Lambda^*} \psi_k)_{anti-symm}$ and $N_k = 0, 1$).

(c) *Probability* (**N.B.** for *bosons*: $\mu < 0$, since $\varepsilon_k \geq 0$) :

$$\mathrm{Pr}_{\beta,\mu}(N_k) := e^{-\beta(\varepsilon_k - \mu) N_k} / \Xi_k(\beta, \mu) \ , \ k \in \Lambda^*.$$

(d) *Expectation* of occupation number for $k \in \Lambda^*$:

$$\mathbb{E}_{\beta,\mu}(N_k) = \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} \ .$$

(e) Mean value of the *total* density of bosons in Λ:

$$\rho_\Lambda(\beta, \mu) := \mathbb{E}_{\beta,\mu}(N/V) = \frac{1}{V} \sum_{k \in \Lambda^*} \mathbb{E}_{\beta,\mu}(N_k) \ .$$

1.1 Conventional BEC: grand-canonical ensemble (β, μ)

• [Uhlenbeck(1927)] *Dual set* Λ^* of momenta w.r.s. to $(-\Delta/2)_{\mathbf{p.b.}}$

$$\Lambda^* := \{k_j := \frac{2\pi}{V^{\alpha_j}} n_j : n_j \in \mathbb{Z}\}_{j=1}^{d=3} \quad \text{and} \quad \varepsilon_k := \sum_{j=1}^{d} k_j^2/2$$

• **Cube**: $\alpha_1 = \alpha_2 = \alpha_3 = 1/3$, $V = L^3$. If $\mu < 0$ (!) and $\Lambda \nearrow \mathbb{R}^3$:

$$\begin{aligned}
\rho(\beta,\mu) &= \lim_{\Lambda} \rho_\Lambda(\beta,\mu) := \lim_{\Lambda} \frac{1}{V}\{\frac{1}{e^{-\beta\mu}-1} + \sum_{k\in\{\Lambda^*\setminus\{0\}\}} \frac{1}{e^{\beta(\varepsilon_k-\mu)}-1}\} \\
&= \lim_{L\to\infty} \frac{1}{L^3} \sum_{n_j\in\mathbb{Z}\setminus\{0\}} \left\{e^{\beta(\sum_{j=1}^{d}(2\pi n_j/V^{1/3})^2/2-\mu)} - 1\right\}^{-1} \\
&= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} d^3k \left\{e^{\beta(k^2/2-\mu)} - 1\right\}^{-1} =: \mathfrak{I}_3(\beta,\mu) \nearrow \mathfrak{I}_3(\beta,0),
\end{aligned}$$

for $\mu \nearrow 0$.

Controversy: Uhlenbeck/Einstein. PBG has no sense ?

- For **d** > 2 the *Perfect* Bose-Gas *maximal density* is **bounded**:

$$\rho_c(\beta) := \lim_{\mu \nearrow 0} \mathfrak{I}_d(\beta,\mu) = \int_0^\infty \frac{C_d\, E^{d/2-1}\, dE}{e^{\beta E}-1} < \infty \ .$$

No more bosons are allowed in the system ? [Uhlenbeck 1927]

- [Einstein 1925] **If** $\rho > \rho_c(\beta)$ (critical density), then by some **saturation mechanism** (?) one gets a **condensate** at $k=0$ (ground-state, $\varepsilon_0 = 0$):

$$\rho_0(\beta) := \rho - \rho_c(\beta) \ .$$

N.B. "Solution" of the Einstein-Uhlenbeck controversy (1925-27) by F.London only in 1938 is due to :

- Elucidation of equation: $\rho = \rho_\Lambda(\beta,\mu)$, in the **thermodynamic limit** (1937) for any fixed ρ.
- Analysis of the "scaling limit" for solutions: $\mu_\Lambda(\beta,\rho)$.

1.2 Saturation Mechanism (the *Conventional* **BEC**):
[F.London(1938)] Let $\mu_\Lambda(\beta,\rho)$ be solution of the equation

$$\rho = \rho_\Lambda(\beta,\mu) \quad \Leftrightarrow \quad \rho \equiv \rho_\Lambda(\beta,\mu_\Lambda(\beta,\rho)) \qquad ('' scaling'' \;\; solution).$$

- $\lim_\Lambda \; \mu_\Lambda(\beta,\rho<\rho_c(\beta)) = \mu(\beta,\rho) < 0$, or
- $\lim_\Lambda \; \mu_\Lambda(\beta,\rho\geq\rho_c(\beta)) = 0$, and

$$\rho_0(\beta) = \rho - \rho_c(\beta) = \lim_\Lambda \frac{1}{V} \; \left\{e^{-\beta\,\mu_\Lambda(\beta,\rho\geq\rho_c(\beta))} - 1\right\}^{-1} > 0 \Rightarrow$$

$$\mu_\Lambda(\beta,\rho\geq\rho_c(\beta)) = -\frac{1}{V}\;\frac{1}{\beta(\rho-\rho_c(\beta))} + o(1/V) \; .$$

- Since $\varepsilon_k = \sum_{j=1}^{d}(2\pi n_j/V^{1/3})^2/2$, the **condensate** exists **ONLY** in **k=0**-mode:

$$\lim_\Lambda \frac{1}{V}\left\{e^{\beta(\varepsilon_{k\neq 0}-\mu_\Lambda(\beta,\rho))} - 1\right\}^{-1} = 0 \; ,$$

- This is a well-known *conventional* (**type I**) BEC.

1.3 Saturation Mechanism (*Generalised* BEC of **type II**):

• **The Casimir Box (1968):** Let $\alpha_1 = 1/2$, i.e. $\alpha_2 + \alpha_3 = 1/2$. Since $\varepsilon_{k_1,0,0} = (2\pi n_1/V^{1/2})^2/2 \sim 1/V$, then again the solution of

$$\rho = \rho_\Lambda(\beta,\mu) \quad \Leftrightarrow \quad \rho \equiv \rho_\Lambda(\beta,\mu_\Lambda(\beta,\rho)).$$

has asymptotics $\mu_\Lambda(\beta,\rho \geq \rho_c(\beta)) = -A/V + o(1/V)$, $A \geq 0$, although the number of modes producing condensate is **infinite !**

• Generalised **type II** BEC [van den Berg-Lewis-Pulé (1978)]:

$$\begin{aligned} \rho - \rho_c(\beta) &= \lim_{L\to\infty} \frac{1}{V} \sum_{n_1 \in \mathbb{Z}} \left\{ e^{\beta((2\pi n_1/V^{1/2})^2/2 - \mu_\Lambda(\beta,\rho))} - 1 \right\}^{-1} \\ &= \sum_{n_1 \in \mathbb{Z}} \frac{1}{(2\pi n_1)^2/2 + A} \, . \end{aligned} \qquad (1)$$

Here $A \geq 0$ is a *unique root* of equation (1).

• **N.B.** The **type II** is infinitely *fragmented* quasi-condensate.

• **The van den Berg-Lewis-Pulé Box:** $\alpha_1 > 1/2$.

• **Proposition 1.2**[van den Berg-Lewis-Pulé (1978)] Let $\alpha_1 > 1/2$, $\alpha_2 + \alpha_3 < 1/2$. Then one gets the Generalised BEC of **type III**, i.e., there is **no** macroscopic occupation of **any** level :

$$\lim_{\Lambda} \frac{1}{V} \left\{ e^{\beta(\varepsilon_k - \mu_\Lambda(\beta,\rho))} - 1 \right\}^{-1} = 0, \quad k \in \Lambda^* .$$

• **Definition 1.3** (generalised BEC of types I, II, or III)

$$\rho - \rho_c(\beta) := \lim_{\eta \to +0} \lim_{\Lambda} \frac{1}{V} \sum_{\{k \in \Lambda^*, \|k\| \leq \eta\}} \left\{ e^{\beta(\varepsilon_k - \mu_\Lambda(\beta,\rho))} - 1 \right\}^{-1} \geq 0 \ .$$

• **Saturation** and ρ_m-**PROBLEM**: [*van den Berg-Lewis-Pulé*] Is it possible that for $\rho \in (\rho_c, \rho_m)$ one has **type III (or II) BEC** and then **type I**, for $\rho \geq \rho_m$? **Yes!** [BEC with the Second Critical Point ρ_m / T_m in **"cigar" traps**, Beau-Zagrebnov (2010)].

2.1 Zero-Mode Condensate and the Bogoliubov Weakly Imperfect Bose Gas: Theory of Superfluidity (1947)

• Let **interacting** bosons be enclosed in a *cubic* box $\Lambda = L \times L \times L \subset \mathbb{R}^3$ of the volume $V \equiv |\Lambda| = L^3$, with (*for simplicity*) periodic boundary (p.b.) conditions on $\partial\Lambda$.

• $\varphi(x)$ is a two-body potential with Fourier transformation:

$$v(q) = \int_{\mathbb{R}^3} d^3x \ \varphi(x) \, e^{-iqx}, \ \ q \in \mathbb{R}^3.$$

• **Suppose** [Bogoliubov (1947)] that the two-body interaction potential $\varphi(x)$ is such that:

(A) $\varphi(x) = \Phi(\|x\|)$ (*isotropic*) and $\varphi \in \mathcal{L}^1(\mathbb{R}^3)$.

(B) $v(k)$ is a (*real continuous*) function, satisfying $v(0) > 0$ and $0 \leq v(k) \leq v(0)$ for $k \in \mathbb{R}^3$.

• Let $\mathcal{F}_b := \mathcal{F}_{symm}(\mathcal{L}^2(\Lambda))$ be the boson Fock space over $\mathcal{L}^2(\Lambda)$ and the CCR creation and annihilation operators:

$$a_k^* := a(\psi_k)^*,\, a_k = a(\psi_k), \quad [a_k, a_{k'}^*] = \delta_{k,k'}\,, \quad k, k' \in \Lambda^*,$$

for eigenvectors $\{\psi_k\}_{k\in\Lambda^*}$ of the one-particle *kinetic-energy* operator $t_\Lambda = (-\Delta/2)_{p.b.}$.

• The **second quantisation** of operators t_Λ and $\varphi(\cdot)$:

$$T_\Lambda := d\Gamma(t_\Lambda) = \sum_{k\in\Lambda^*} \varepsilon_k a_k^* a_k\ , \quad N_\Lambda = \sum_{k\in\Lambda^*} a_k^* a_k$$

$$U_\Lambda := d\Gamma(\varphi(\cdot)) = \frac{1}{2V} \sum_{k_1,k_2,q\in\Lambda^*} v(q)\, a_{k_1+q}^* a_{k_2-q}^* a_{k_2} a_{k_1}$$

• Then $H_\Lambda = T_\Lambda + U_\Lambda$, $\mathrm{Dom}(H_\Lambda) \subset \mathcal{F}_b$, is a self-adjoint semi-bounded from below **Hamiltonian** of **Imperfect Bose-Gas**.

- The **Imperfect Bose-Gas** and **Bose condensate**:

- The Hamiltonian *in* the boson Fock space $\mathcal{F}_b$:

$$H_\Lambda = \sum_{k\in\Lambda^*} \varepsilon_k \, a_k^* a_k + \frac{1}{2V} \sum_{k_1,k_2,q\in\Lambda^*} v\,(q)\, a_{k_1+q}^* a_{k_2-q}^* a_{k_2} a_{k_1} \,.$$

- The grand-canonical **Gibbs expectations** $\mathbb{E}_{\beta,\mu}^{\Lambda}(A)$ for $A \in \mathfrak{A}$:

$$\mathbb{E}_{\beta,\mu}^{\Lambda}(A) = (\Xi_\Lambda\,(\beta,\mu))^{-1}\mathrm{Tr}_{\mathcal{F}_b}\,(e^{-\beta(H_\Lambda-\mu N_\Lambda)}\,A)\,,$$

where partition function $\Xi_\Lambda\,(\beta,\mu) = \mathrm{Tr}_{\mathcal{F}_b}\, e^{-\beta(H_\Lambda-\mu N_\Lambda)}$. and the **grand-canonical pressure** is $p_\Lambda\,[H_\Lambda]\,(\beta,\mu) = (\beta\, V)^{-1} \ln \Xi_\Lambda\,(\beta,\mu)$,
- Given that $N_0 := a_0^* a_0$ is the particle-number operator for $k = 0$, the zero-mode (conventional / non-conventional) **condensate** density at (β,μ) exists if (still an **open problem**)

$$\rho_0\,(\beta,\mu) := \lim_{V\to\infty} \frac{1}{V}\, \mathbb{E}_{\beta,\mu}^{\Lambda}(a_0^* a_0) > 0\,.$$

2.2 Weakly Imperfect Bose-Gas: Hamiltonian H_Λ^B (1998)

- Suppose that condensation in the mode $k = 0$ **persists** for a *weak* interaction $\varphi(x)$, then Bogoliubov suggested (1947) to **truncate** H_Λ and to keep **only** the *most important* terms, in which at least **two** operators a_0^*, a_0 from condensate are involved.
- This is the Bogoliubov Weakly Imperfect Bose-Gas (WIBG):

$$H_\Lambda^B := T_\Lambda + U_\Lambda^D + U_\Lambda^{ND} + \frac{v(0)}{2V}\ a_0^* a_0^*\, a_0\, a_0\,, \quad v(0) > \mathbf{0},$$

$$U_\Lambda^D := \frac{v(0)}{V} a_0^* a_0 \sum_{k \in \Lambda^* \setminus \{0\}} a_k^* a_k + \sum_{k \in \Lambda^* \setminus \{0\}} \frac{v(k)}{2} \frac{a_0^* a_0}{V} (a_k^* a_k + a_{-k}^* a_{-k})$$

$$U_\Lambda^{ND} := \frac{1}{2V} \sum_{k \in \Lambda^* \setminus \{0\}} v(k) (a_k^* a_{-k}^*\, a_0 a_0 + a_0^* a_0^*\, a_k a_{-k})\ .$$

N.B. Instability of Bose-gas w.r.t. particle attraction: $v(0) < \mathbf{0}$.

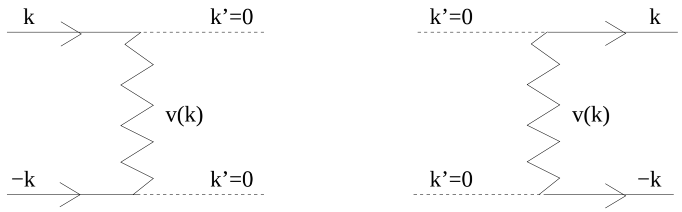
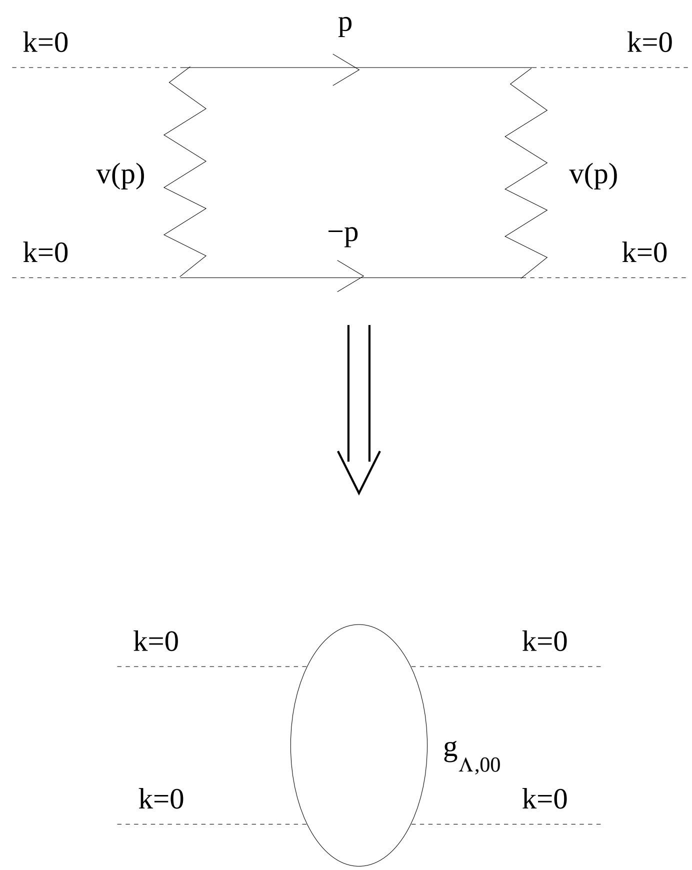


Figure 2.3

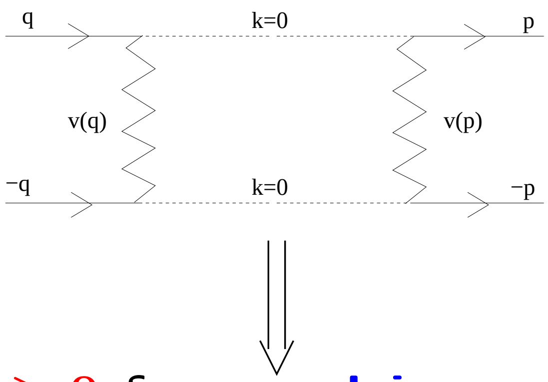
Vertices corresponding to the **Non-Diagonal** interaction :

$$U_{\Lambda}^{ND} := \frac{1}{2V} \sum_{k \in \Lambda^* \setminus \{0\}} v(k) \ (a_0^* \, a_0^* \ a_k a_{-k} + a_k^* a_{-k}^* \ a_0 \, a_0) \ .$$



The effective vertex $g_{\Lambda,00} < 0$ for **attraction** between particles **in** condensate. Total interaction = (direct + effective) vertices:

$$\mathbf{Q}: \quad \frac{v(0)}{2} + g_{00} < \mathbf{0} \quad ? \quad \textbf{Yes!}$$



Effective vertex $\mathbf{g_{\Lambda,pq} \geq 0}$ for **repulsion** **outside** condensate.

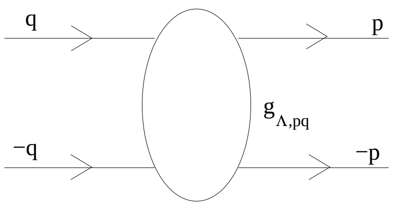


Figure 3.1

• **Proposition [BZ]** If $v(0)/2 + g_{00} < 0$, then WIBG manifests **two** different kinds of Bose condensation $\rho_0^B(\beta, \mu)$, $d \geq 1$ (!):

- The **first** kind, for $0 > \mu > \mu_0(\theta = \beta^{-1})$, due to **attraction** between bosons in the mode **k=0** (**non-conventional** *dynamical* Bose-condensation) if $\theta < \theta_c(\mu = 0) =: \theta_0$.

- The **second** kind, for $\mu = 0$, is the **conventional** Bose-Einstein condensation due to the **saturation** mechanism.

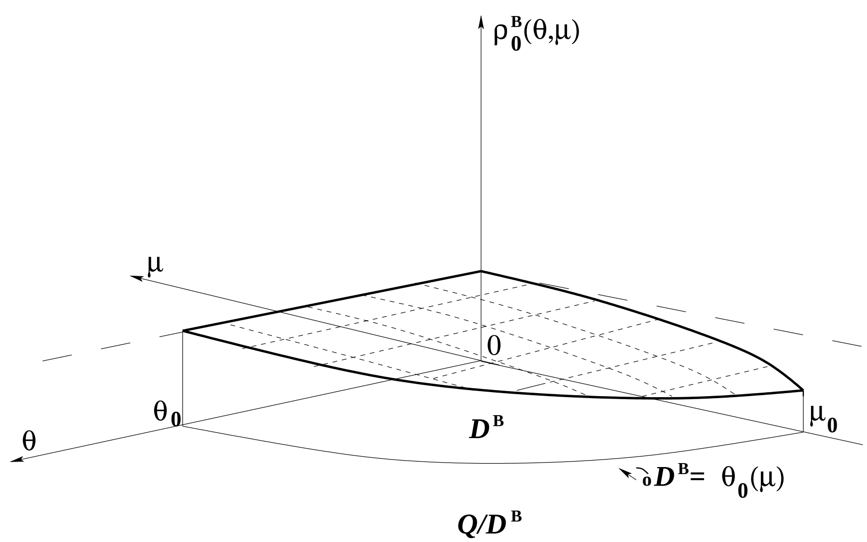
In this large-density regime the **non-conventional** condensate and the **conventional** BEC in the Bogoliubov Weakly Imperfect Bose-Gas *coexist*, cf. Perfect Bose-Gas for $\mu \leq 0$, $d > 2$.

- One gets for $\mu \leq 0$ and $d \geq 1$ the pressure:

$p^B(\beta, \mu) := \lim_\Lambda p_\Lambda \left[T_\Lambda + U_\Lambda^D + \frac{v(0)}{2V}\ {a_0^*}^2 {a_0}^2 + U_\Lambda^{ND} \right] (\beta, \mu) \neq p^{PBG}(\beta, \mu)$

with *equality* if $\{v(\cdot) = 0 \vee \rho_0^B(\beta, \mu) = 0\}$. **Note** that

$$\lim_\Lambda p_\Lambda \left[T_\Lambda + U_\Lambda^D + \frac{v(0)}{2V}\ {a_0^*}^2 {a_0}^2 + \mathbf{0} \right] = \lim_\Lambda p_\Lambda \left[T_\Lambda \right] =: p^{PBG} \ \mathbf{!}$$


$\rho_0^B(\theta,\mu)$
μ
0
θ
θ_0
μ_0
D^B
$\partial D^B = \theta_0(\mu)$
Q/D^B

2.3 Huang-Yang-Luttinger model (1957-1988)

• Let $N_\Lambda := \sum_{k\in\Lambda^*} N_k$ and $T_\Lambda := \sum_{k\in\Lambda^*} \varepsilon_k N_k$, where $N_k := a_k^* a_k$. Then Hamiltonian of **diagonal** HYL-model for $\lambda > 0$

$$H_\Lambda^{HYL} := T_\Lambda + \frac{\lambda}{2V}\{N_\Lambda^2 - \sum_{k\in\Lambda^*} N_k^2\} + \frac{g}{2V} N_\Lambda^2, \quad g > 0.$$

• Since $(N_\Lambda^2 - \sum_{k\in\Lambda^*} N_k^2) \geq 0$ the **interaction** is minimal $(= 0)$ when **all** particles occupy a **single** energy-level, e.g., $N_k = N_\Lambda$.

• Since $\varepsilon_k = \hbar^2 k^2/2m$, a minimum $(= 0)$ of the **kinetic-energy** term $T_\Lambda \geq 0$ selects for **all** particles the **zero-mode** level $k = 0$.

• **Proposition [van den Berg, Dorlas, Lewis, Pulè (1990)]**
If $\lambda > 0$, the HYL-model manifests for $\mu > \mu_0(\theta, \lambda)$, where $\mu \in \mathbb{R}$! and $d \geq 1$, a **non-conventional** condensation in the **mode** $k = 0$.

• For $\lambda = 0$ the non-conventional condensation **disappears**, although then model (**MF** Bose-gas) manifests for $d > 2$ the **conventional** BEC in the **mode** $k = 0$.

THANK YOU FOR YOUR ATTENTION !

https://www.sciencedirect.com/science/article/abs/pii/S0370157300001320

https://link.springer.com/article/10.1134/S106377962102009X

2.4 Stable Weakly Imperfect Bose-Gas [AB](2004), [BZ](2008)

- The: $U^D \to U_\Lambda^{SD}$ is **stabilised** ($\mu \in \mathbb{R}$) by the Mean-Field term:

$$H_\Lambda^{SB} := T_\Lambda + U_\Lambda^{SD} + \mathbf{U}_\Lambda^{\mathbf{ND}} + \frac{v(0)}{2V}\, a_0^* a_0^* a_0 a_0 \,, \quad v(0) > \mathbf{0},$$

$$U_\Lambda^{SD} := \frac{v(0)}{2V} \sum_{\{k' \vee k\} \in \Lambda^* \setminus \{0\}} a_{k'}^* a_{k'} a_k^* a_k + \sum_{k \in \Lambda^* \setminus \{0\}} \frac{v(k)}{2} \frac{a_0^* a_0}{V} (a_k^* a_k + a_{-k}^* a_{-k})\,.$$

As a result one infers for $N_\Lambda := \sum_{k \in \Lambda^*} a_k^* a_k$ that

$$H_\Lambda^{SB} := T_\Lambda + \sum_{k \in \Lambda^* \setminus \{0\}} \frac{v(k)}{2} \frac{a_0^* a_0}{V} (a_k^* a_k + a_{-k}^* a_{-k}) + \mathbf{U}_\Lambda^{\mathbf{ND}} +$$

$$+ \frac{v(0)}{2V}\, N_\Lambda^2 - \frac{v(0)}{2V}\, a_0^* a_0 \,, \quad v(0) > \mathbf{0}\,.$$