The condensate fraction

Let $Q \subset \mathbb{R}^3$ be a box with periodic boundary conditions, i.e. Q is a torus. Let $N \in \mathbb{N}$ be the number of particles and let the interaction potential be given by a function $v: \mathbb{R}^3 \longrightarrow [0,\infty)$, v radial, $(1+|x|^4)v \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. We consider the Hamiltonian

$$H := \underbrace{\frac{1}{2}\sum_{i=1}^{N}(-\Delta_{x_i})}_{\text{kinetic energy term}} + \underbrace{\sum_{i<j} v(x_i - x_j)}_{\text{interaction term}} \quad \text{on} \quad L^2_{sym.}(Q^N)$$

We only look at symmetric wave functions because we consider bosons

Fact: H has a unique ground state Ψ with $\|\Psi\|_{L^2}=1$ and $\Psi \geq 0$
[This follows from the diamagnetic inequality].

For $N=1$ (i.e. the interaction term vanishes), the ground state is given by the constant function $\frac{1}{\sqrt{|Q|}} \in L^2(Q)$. We call this function the condensate wave function.

Question: In the ground state Ψ, which fraction of the particles is not in the condensate? That is, we want to compute

$$1 - \underbrace{\frac{1}{N}\sum_{j=1}^{N}\langle \Psi, P_j \Psi\rangle}_{\substack{\text{fraction of particles} \\ \text{in the condensate}}} = \langle \Psi, \underbrace{\left(\mathbb{1} - \frac{1}{N}\sum_{j=1}^{N} P_j\right)}_{=:A} \Psi\rangle,$$

where P_j denotes the projection on the condensate wave function $\frac{1}{\sqrt{|Q|}}$ in the j^{th} particle:

$$(P_j\Phi)(x_1,\dots,x_N) := \int_Q dx_j \frac{1}{|Q|}\Phi(x_1,\dots,x_N) \quad \text{for } \Phi \in L^2_{sym.}(Q^N).$$

<u>Problem</u>: We don't have good information on Ψ, which makes it difficult to compute $\langle \Psi, A\Psi \rangle$ directly. However, we have relatively good control of the energy.

<u>Hellmann - Feynman argument</u>

For $\mu \in \mathbb{R}$, define the operator

$$H_\mu := H + \mu A$$

Let E_μ be the ground state energy of H_μ and let $\Psi_\mu \in L^2_{sym}(Q^N)$ be a ground state of H_μ with $\|\Psi_\mu\| = 1$ and $\langle \Psi_\mu, \Psi \rangle \geq 0$.

<u>Fact</u>: H has a spectral gap, i.e. $\exists c > 0 \ \forall \Phi \in L^2_{sym}(Q^N), \|\Phi\| = 1, \Phi \perp \Psi$:

$$\langle \Phi, H\Phi \rangle - E \geq c.$$

A is a bounded operator. Therefore, $\|H_\mu - H\| = \|H + \mu A - H\| \leq |\mu| \, \|A\| \xrightarrow{\mu \to 0} 0$. We get $E_\mu \xrightarrow{\mu \to 0} E$. Moreover, since H has a spectral gap, we also know that H_μ has a spectral gap for μ sufficiently close to 0. Since Φ_μ is chosen s.t. $\langle \Psi_\mu, \Psi \rangle \geq 0$, we get $\Psi_\mu \xrightarrow{\mu \to 0} \Psi$ weakly in $L^2_{sym}(Q^N)$.

We have

$$(E_\mu - E)\langle \Psi_\mu, \Psi \rangle = \langle E_\mu \Psi_\mu, \Psi \rangle - \langle \Psi_\mu, E\Psi \rangle \overset{\substack{H_\mu \Psi_\mu = E_\mu \Psi_\mu \\ H\Psi = E\Psi}}{=} \langle H_\mu \Psi_\mu, \Psi \rangle - \langle \Psi_\mu, H\Psi \rangle$$

$$\underset{H_\mu \text{ symm.}}{=} \langle \Psi_\mu, H_\mu \Psi \rangle - \langle \Psi_\mu, H\Psi \rangle \underset{H_\mu = H + \mu A}{=} \langle \Psi_\mu, (H + \mu A)\Psi \rangle - \langle \Psi_\mu, H\Psi \rangle = \mu \langle \Psi_\mu, A\Psi \rangle.$$

Therefore, for $\mu \neq 0$ small enough (note: $\langle \Psi_\mu, \Psi \rangle > 0$ for μ suff. small),

$$\frac{E_\mu - E}{\mu} = \frac{\langle \Psi_\mu, A\Psi \rangle}{\langle \Psi_\mu, \Psi \rangle} \xrightarrow[\Psi_\mu \rightharpoonup \Psi]{\mu \to 0} \frac{\langle \Psi, A\Psi \rangle}{\langle \Psi, \Psi \rangle} \underset{\|\Psi\| = 1}{=} \langle \Psi, A\Psi \rangle$$

This is what we want to compute

Thus, $\mu \mapsto E_\mu$ is differentiable at 0 and we have

$$\boxed{\left.\frac{d}{d\mu}\right|_{\mu = 0} E_\mu = \langle \Psi, A\Psi \rangle}$$

The modified simple equation

The simple equation corresponding to the Hamiltonian H_μ is called the modified simple equation, which is given by

$$
\text{(MSE)}\begin{cases} (-\Delta+2\mu+4e_\mu)u_\mu = (1-u_\mu)v + 2\rho\, e_\mu\, u_\mu * u_\mu \\ e_\mu = \frac{\rho}{2}\int_{\mathbb{R}^3} dx\,(1-u_\mu)v \end{cases} \quad \text{on } \mathbb{R}^3,
$$

where $\rho>0$ corresponds to the particle density

e_μ corresponds to the energy per particle.

We want to compute $\frac{d}{d\mu}\Big|_{\mu=0} e_\mu =: \eta$ for small ρ. We think of η as the fraction of the particles outside the condensate (compare with the Hellmann-Feynman argument).

Notation :

$u := u_0$ solution to the simple equation ($\mu=0$).

$e := e_0$

$K_e := (-\Delta+V+4e(1-C_{\rho u}))^{-1}$ convolution operator with ρu

a : scattering length of v

Theorem (Condensate fraction for $\rho\to 0$) (Th. 1.7)

We have

$$\eta = \frac{\rho\int dx\, v K_e u}{1-\rho\int dx\, v\, K_e[2u-\rho u*u)}$$

Moreover,

$$\eta = \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}} + o(\sqrt{\rho}) \quad \text{as } \rho\to 0.$$

Some facts, which we will use in the proof

Lemma 1.11 (Properties of K_e)

- Boundedness $L^1 \longrightarrow L^2$: $\forall e>0\ \forall \psi \in L^1(\mathbb{R}^3)$: $\|K_e\psi\|_2 \leq \frac{1}{\pi}(2e)^{-1/4}\|\psi\|_1$
- Symmetry: $\forall \varphi, \psi \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$: $\int dx\, \varphi(K_e\psi) = \int dx\, (K_e\varphi)\psi$
- $\forall x \in \mathbb{R}^3\ \forall e \geq 0$: $0 \leq (K_e v)(x) \leq 1$

  interaction potential

Other useful facts

- $\forall x \in \mathbb{R}^3$: $0 \leq u(x) \leq 1$ [I, (1.6)] and $\int_{\mathbb{R}^3} dx\, u(x) = \frac{1}{\varrho}$ [I, (1.7)]
- $\|u\|_2 \leq \dfrac{e^{-1/4}}{4\sqrt{\pi}}\|v\|_1$ [(1.24)]
- $e = 2\pi \varrho a + o(\varrho)$ as $\varrho \to 0$ [I, Th. 1.4]
- For $e>0$ small enough, the map $e \mapsto \varrho(e)$ is C^1 and strictly mon. increasing. [Th. 1.4]
- The solution to (MSE) $(u_\mu, e_\mu) \in (L^2(\mathbb{R}^3), [0,\infty))$ exists and it is differentiable wrt μ. [comment on p. 19]
- As an operator on $L^2(\mathbb{R}^3)$, $0 \leq 1 - C_{\varrho u} \leq 2$ [$\Rightarrow K_e$ is well-def. for all $e \geq 0$] [(1.38)]
- For $e>0$ small enough, there exists a constant $C>0$ indep. of e s.t. $\forall\, 1<q<p<\infty$, $\frac{1}{p} = \frac{1}{q} - \frac{1}{3}$: $\|K_e\psi\|_q \leq C e^{-1/2}\|\psi\|_p$ $\forall \psi \in L^p$.

  [see p. 10]

Proof of the theorem on the condensate fraction:

Step 1: $\eta = \dfrac{\rho \int dx\, v\, K_e u}{1 - \rho \int dx\, v\, K_e(2u - \rho u * u)}$ if the denominator is $\neq 0$.

Define / recall:

$$\eta = \frac{d}{d\mu}\Big|_{\mu=0} e_\mu = e'_\mu|_{\mu=0} \qquad e = e_\mu|_{\mu=0}$$

$$s := \frac{d}{d\mu}\Big|_{\mu=0} u_\mu = u'_\mu|_{\mu=0} \qquad u = u_\mu|_{\mu=0}$$

Differentiate the first equation of (MSE) $\underbrace{}_{\text{wrt. } \mu}$ to get

$$(-\Delta + 2\mu + 4e_\mu) u'_\mu + (2 + 4e'_\mu) u_\mu = -u'_\mu v + 2\rho e'_\mu u_\mu * u_\mu$$
$$+ 4\rho e_\mu u_\mu * u'_\mu$$

and evaluate at $\mu = 0$ to get

$$(-\Delta + 4e)s + (2 + 4\eta)u = -sv + 2\rho\eta\, u*u + 4\rho e\, u*s$$

We obtain

$$(-\Delta + v + 4e(1 - C_{\rho u}))s = -2u - 4\eta u + 2\rho\eta\, u*u,$$

which implies

$$s = K_e(-2u - 4\eta u + 2\rho\eta\, u*u) \qquad (*)$$

Differentiating the second equation of (MSE) wrt. μ and evaluating at $\mu = 0$, we get

$$\eta = \frac{\rho}{2}(-1)\int dx\, s v \overset{(*)}{=} -\frac{\rho}{2}\int dx\, K_e(-2u - 4\eta u + 2\rho\eta\, u*u)\, v$$

$$\overset{\substack{\text{symmetry}\\ \text{of } K_e}}{=} \rho \int dx\, (K_e v)\,(u + 2\eta u - \rho \eta\, u*u)$$

and therefore,

$$\eta\underbrace{\left(1 - \rho \int dx\, (K_e v)(2u - \rho\, u*u)\right)}_{\varsigma} = \rho \int dx (K_e v) u$$

Now, if $\varsigma \neq 0$, we get

$$\eta = \frac{\rho \int dx\, (K_e v) u}{1 - \rho \int dx\, (K_e v)(2u - \rho\, u*u)},$$

which is what we wanted to show by the symmetry of K_e.

<u>Step 2</u>: Strategy for the rest of the proof

Define

$$X := \rho \int dx\, (K_e v) u$$
$$Y := \rho^2 \int dx\, (K_e v)(u*u)$$

We will show:

$$X = O(\sqrt{\rho}) \text{ as } \rho \to 0$$
$$Y = O(\sqrt{\rho}) \text{ as } \rho \to 0$$

By step 1, we know that

$$\eta = \frac{X}{1-2X+Y} = X + \underbrace{\underbrace{X}_{=O(\sqrt{\rho})}\Big(\underbrace{\frac{1}{1-2X+Y} - 1}_{=o(1)}\Big)}_{=o(\sqrt{\rho})} = X + o(\sqrt{\rho}) \quad \text{as } \rho \to 0.$$

Thus, in order to show $\eta = C\sqrt{\rho} + o(\sqrt{\rho})$ as $\rho \to 0$ for some $C>0$, it suffices to show $X = C\sqrt{\rho} + o(\sqrt{\rho})$ and $Y = O(\sqrt{\rho})$ as $\rho \to 0$.

Step 3: $Y = \mathcal{O}(\sqrt{\varrho})$ as $\varrho \to 0$

We have

$$|Y| = \varrho^2 \left| \int dx\, (K_e v)\, (u * u) \right| \overset{\text{Cauchy-Schwarz}}{\leq} \varrho^2 \, \|K_e v\|_2 \, \underbrace{\|u * u\|_2}_{\substack{\leq \|u\|_2 \|u\|_1 \text{ (Young's ineq.)} \\ = \|u\|_2 \frac{1}{\varrho}}}$$

$$\leq \varrho \, \|K_e v\|_2 \, \|u\|_2 \overset{\text{facts on p.4}}{\leq} \varrho \left(\frac{1}{\pi} (2e)^{-1/4} \|v\|_1 \right) \left(\frac{e^{-1/4}}{4\sqrt{\pi}} \|v\|_1 \right)$$

$$= C \varrho e^{-1/2} \|v\|_1^2 \underset{\substack{\uparrow \\ \text{as } \varrho \to 0 \\ e = 2\pi\varrho a + o(\varrho)}}{=} C \|v\|_1^2 \, \varrho \, \mathcal{O}(\varrho^{-1/2}) = \mathcal{O}(\sqrt{\varrho}) \quad \text{as } \varrho \to 0$$

Step 4: $X = \dfrac{8\sqrt{a^3}}{3\sqrt{\pi}} \sqrt{\varrho} + o(\sqrt{\varrho})$ as $\varrho \to 0$

First, we would like to re-write $X = \varrho \int dx (K_e v) u$ in terms of a new function ξ. Recall the resolvent identity

$$\frac{1}{A+B} - \frac{1}{A} = - \frac{1}{A+B} B \frac{1}{A} .$$

We have

$$K_e = \big(\underbrace{-\Delta + 4e(1 - C_{\varrho u})}_{=: A} + \underbrace{v}_{=: B} \big)^{-1} = \frac{1}{A+B}$$

$$Y_e := \left(-\Delta + 4e(1 - C_{\varrho u}) \right)^{-1} = \frac{1}{A}$$

Thus,

$$K_e(\varrho u) = \underbrace{Y_e(\varrho u)}_{=: \xi} - K_e [v \, Y_e(\varrho u)] = \xi - K_e(v\xi) , \quad (**)$$

so we get

$$X = \varrho \int dx\, (K_e v) u \overset{\text{symm}}{=} \int dx\, v \, K_e(\varrho u) \overset{(**)}{=} \int dx\, v\xi - \int dx\, v \, K_e(v\xi)$$

$$\underset{\substack{\uparrow \\ \text{symm.}}}{=} \int dx\, v\xi - \int dx\, (K_e v) v \xi = \int dx\, v\xi \, [1 - K_e v]$$

Fact: $\xi(x) = \frac{\sqrt{2e}}{3\pi^2} + o(\sqrt{e})$ as $e \to 0$ unif. in $x \in \mathbb{R}^3$.

We obtain

$$X = \left(\frac{\sqrt{2e}}{3\pi^2} + o(\sqrt{e})\right)\underbrace{\left(\int dx\, v\,[1 - K_e v]\right)}_{\cdot \leq \int dx\, v(x) < \infty \quad \text{since } 0 \leq (K_e v)(x) \leq 1 \ \forall x \in \mathbb{R}^3}$$

$$= \frac{\sqrt{2e}}{3\pi^2}\int dx\, v\,[1 - K_e v] + o(\sqrt{e}) \quad \text{as } e \to 0$$

Claim: $\int dx\, v\, K_e v \xrightarrow{e \to 0} \int dx\, v\, (-\Delta + v)^{-1} v$

Suppose the claim was true. We get

$$X = \frac{\sqrt{2e}}{3\pi^2}\left(\int dx\, v - \int v\, K_e v\right) + o(\sqrt{e})$$

$$\overset{\text{claim}}{=} \frac{\sqrt{2e}}{3\pi^2}\left(\int dx\, v - \int v\,(-\Delta + v)^{-1} v + o(1)\right) + o(\sqrt{e})$$

$$= \frac{\sqrt{2e}}{3\pi^2}\underbrace{\int dx\, v\,[1 - (-\Delta + v)^{-1} v]}_{= 4\pi a} + o(\sqrt{e})$$

one of the definitions of the scattering length [I, (4.12)]

$$= \frac{4a\sqrt{2e}}{3\pi} + o(\sqrt{e}) \underset{e = 2\pi\rho a + o(\rho)}{=} \frac{4a\sqrt{2}}{3\pi}\sqrt{2\pi\rho a} + o(\sqrt{\rho})$$

$$= \frac{8}{3\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho}). \quad \text{as } \rho \to 0.$$

Thus,

$$\eta = X + o(\sqrt{\rho}) = \frac{8}{3\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho}) \quad \text{as } \rho \to 0.$$

It remains to show the claim. By the resolvent identity,

$$K_e = (\underbrace{-\Delta + v}_{=:A} + \underbrace{4e(1 - C_{\rho u})}_{=:B})^{-1} = \frac{1}{A+B}$$

$$(-\Delta + v)^{-1} = \frac{1}{A}$$

$$K_e - (-\Delta+v)^{-1} = \frac{1}{A+B} - \frac{1}{A} = -\frac{1}{A+B} B \frac{1}{A} = -K_e 4e(1-C_{gu})(-\Delta+v)^{-1},$$

So we get

$$\left| \int dx\, v K_e v - \int dx\, v (-\Delta+v)^{-1} v \right| = \left| \int dx\, v (-1) K_e 4e (1-C_{gu})(-\Delta+v)^{-1} v \right|$$

$$\underset{\substack{\uparrow \\ K_e \text{ symm.}}}{=} 4e \left| \int dx\, (K_e v) \cdot (1-C_{gu})(-\Delta+v)^{-1} v \right|$$

$$\underset{\substack{\uparrow \\ \text{Hölder} \\ 1=\frac{5}{6}+\frac{1}{6}}}{\leq} 4e \, \| K_e v \|_{\frac{6}{5}} \, \| (1-C_{gu})(-\Delta+v)^{-1} v \|_6$$

$$\underset{\uparrow}{\leq} 4e\, C e^{-1/2} \|v\|_2 \; 2 \, \|(-\Delta+v)^{-1} v\|_6 = 8C\sqrt{e}\, \|v\|_2 \underbrace{\|(-\Delta+v)^{-1} v\|_6}_{<\infty \text{ because}} \xrightarrow{e\to 0} 0$$

- $\|K_e f\|_q \leq C e^{-1/2} \|f\|_p$ for $\frac{1}{p} = \frac{1}{q} - \frac{1}{3}$.
  Here: $q = \frac{6}{5}$, i.e. $\frac{1}{p} = \frac{5}{6} - \frac{1}{3} = \frac{3}{6} = \frac{1}{2}$, so $p=2$
- $1-C_{gu} : L^6 \to L^6$ bdd. with op. norm ≤ 2

$<\infty$ because $0 \leq [(-\Delta+v)^{-1} v](x) \leq 1$ and $[(-\Delta+v)^{-1} v](x)|x| \xrightarrow{|x|\to\infty} a < \infty$ (def. of a)

$\square$

The condensate fraction in the thermodynamic limit in Bogoliubov theory

Let $N \in \mathbb{N}$ be the number of particles, let $L > 0$ be the size of the box $\Lambda_L := L\mathbb{T}^3$ (torus in $\mathbb{R}^3$ of side length L). Let $w \in C_c^\infty(\mathbb{R}^3), w \geq 0$ be an even function. We consider

$$H := H_{N,L} := \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{\substack{i,j=1 \\ i \neq j}}^{N} w(x_i - x_j) \quad \text{on} \quad L^2_{sym}(\Lambda_L^N)$$

For $p \in 2\pi\mathbb{Z}^3$, define

$$u_p(x) := L^{-3/2} e^{ip\frac{x}{L}} \quad , x \in \Lambda_L$$

and note that $\{u_p\}_{p \in 2\pi\mathbb{Z}^3}$ is an ONB of $L^2(\Lambda_L)$. We call the constant function u_0 the condensate wave function. Note that u_0 is the ground state of $H_{N=1,L}$. We are interested in computing the fraction of particles outside the condensate (i.e. orthogonal to u_0), which is given by

$$\frac{1}{N} \langle \Psi_0, \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} a_p^* a_p \Psi_0 \rangle,$$

where Ψ_0 denotes the ground state of $H_{N,L}$. We are interested in the limit $N \to \infty$, $L \to \infty$, $\frac{N}{L} =: \rho$ of this quantity for small $\rho > 0$. (thermodynamic limit)

Bogoliubov theory [MQM2 p. 137–145]

We think of $H_{N,L}$ as the restriction to the N-particle sector of the bosonic Fock space $\mathcal{F}(L^2(\Lambda_L))$ of the operator

$$\mathbb{H} := \sum_{m,n \in 2\pi\mathbb{Z}^3} h_{mn} a_m^* a_n + \frac{1}{2} \sum_{m,n,p,q \in 2\pi\mathbb{Z}^3} W_{mnpq} a_m^* a_n^* a_p a_q ,$$

where $h_{mn} = \langle u_n, -\Delta u_m \rangle$, $W_{mnpq} := \langle u_m \otimes u_n, w\, u_p \otimes u_q \rangle$

<u>Note</u>: For $p,q\in 2\pi\mathbb{Z}^3$, we have

- $(-\Delta u_p)(x) = \frac{1}{L^2}|p|^2 u_p(x)$. Hence, $h_{m,n} = \frac{|m|^2}{L^2}\delta(m-n)$

- $\langle u_p\otimes u_0, w\, u_0\otimes u_q\rangle = \int_{\Lambda_L} dx \int_{\Lambda_L} dy\, L^{-3/2} e^{-ip\frac{x}{L}} L^{-3/2} w(x-y) L^{-3/2} L^{-3/2} e^{iq\frac{y}{L}}$

$$= \int_{\Lambda_1} dx \int_{\Lambda_1} dy\, \underbrace{e^{-ipx}}_{e^{-ip(x-y)}e^{-ipy}} e^{iqy}\, w(L(x-y)) \underset{x-y=z}{=} \underbrace{\int_{\Lambda_1} dz\, e^{-ipz} \underbrace{w(Lz)}_{=:w_L(z)}}_{=:\hat{w}_L(p)} \underbrace{\int_{\Lambda_1} dy\, e^{i(q-p)y}}_{=\delta(p-q)}$$

$$= \hat{w}_L(p)\,\delta(p-q)$$

- $\langle u_p\otimes u_q, w\, u_0\otimes u_0\rangle = \hat{w}_L(p)\,\delta(p+q)$
- $\langle u_p\otimes u_0, w\, u_q\otimes u_0\rangle = \hat{w}_L(0)\,\delta(p-q)$

Thus,

$$\mathbb{H} = \sum_{p\in 2\pi\mathbb{Z}^3} \frac{1}{L^2}|p|^2 a_p^* a_p + \frac{1}{2}\sum_{m,n,p,q\in 2\pi\mathbb{Z}^3} W_{mnpq}\, a_m^* a_n^* a_p a_q$$

<u>Assumption</u>: For large N, we expect most particles to be in the condensate and we call the number of particles in the condensate N_0.

More precisely, if $\Psi_0^{N,L}$ is the ground state of $H_{N,L}$, then

$$N_0 := N_0^{N,L} := \langle \Psi_0^{N,L}, a_0^* a_0 \Psi_0^{N,L}\rangle$$

and we assume for $\rho>0$ small

$$\lim_{\substack{N,L\to\infty\\ \frac{N}{L}=\rho}} \frac{N_0^{N,L}}{N} = 1 \qquad \text{Bose-Einstein condensation in the thermodynamic limit}$$

⚠ This has not been proven rigorously yet. It is one of the most important problems in mathematical physics.

Bogoliubov's approximation method

Step 1: Ignoring higher order terms

In the second quantisation

$$\mathbb{H} = \sum_{p\in 2\pi\mathbb{Z}^3} \frac{1}{L^2}|p|^2 a_p^* a_p + \frac{1}{2}\sum_{m,n,p,q\in 2\pi\mathbb{Z}^3} W_{mnpq}\, a_m^* a_n^* a_p a_q ,$$

we ignore all terms with three or four $a_n^\#$ for $n\neq 0$ because we expect these terms to be small.

Step 2: c-number substitution

We replace the operators a_0^*, a_0 by $\sqrt{N_0}$. This is motivated by $N_0 = \langle \Psi_0, a_0^* a_0 \Psi_0\rangle$.

Step 3: Cancellation of linear terms

In our case, all terms with exactly one $a_n^\#$ for $n\neq 0$ are zero, since we have already seen that for $n\neq 0$: $W_{n000} = W_{0n00} = W_{00n0} = W_{000n} = 0$.

So far, we have

$$\mathbb{H} \approx \frac{1}{2}\underbrace{W_{0000}}_{=\hat{W}_L(0)} N_0^2 + \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \frac{1}{L^2}|p|^2 a_p^* a_p + \frac{N_0}{2}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \Big\{ \underbrace{W_{p-p00}}_{=\hat{W}_L(p)} a_p^* a_{-p}^*$$

$$+ \underbrace{W_{00p-p}}_{\hat{W}_L(p)} a_p a_{-p} + \big(\underbrace{W_{p00p}}_{\hat{W}_L(p)} + \underbrace{W_{p0p0}}_{\hat{W}_L(0)} + \underbrace{W_{0pp0}}_{\hat{W}_L(p)} + \underbrace{W_{0p0p}}_{\hat{W}_L(0)} \big) a_p^* a_p \Big\}$$

$$\underset{\substack{\uparrow\\ \text{on the N-part.}\\ \text{sector}}}{=} \frac{1}{2}\hat{W}_L(0) \underbrace{\left(N_0^2 + 2N_0(N-N_0)\right)}_{\substack{\approx (N_0+(N-N_0))^2 = N^2\\ \uparrow\\ (N-N_0)^2 \text{ relatively small}}} + \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \left[\frac{1}{L^2}|p|^2 + N_0 \hat{W}_L(p)\right] a_p^* a_p$$

$$+ \frac{N_0}{2}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \hat{W}_L(p)\left(a_p^* a_{-p}^* + a_p a_{-p}\right)$$

Thus, with

$$C_N := \frac{1}{2} \hat{w}_L(0)\, N^2$$

$$\mathbb{H}_{Bog} := \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} \underbrace{\left[\frac{1}{L^2}|p|^2 + N \hat{w}_L(p)\right]}_{=: A_p} a_p^* a_p$$

$$+ \frac{1}{2} \sum_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}} \underbrace{N_0 \hat{w}_L(p)}_{=: B_p} \left(a_p^* a_{-p}^* + a_p a_{-p}\right)$$

using $N_0 \approx N$, we get

$$\mathbb{H} \approx C_N + \mathbb{H}_{Bog}$$

<u>Step 4</u>: Quadratic approximation

For $p \in 2\pi\mathbb{Z}^3 \setminus \{0\}$, define

$$\nu_p = \frac{1}{2}\left(\frac{A_p}{\sqrt{A_p^2 - B_p^2}} - 1\right)$$

and

$$b_p := \sqrt{1+\nu_p^2}\, a_p + \nu_p\, a_{-p}$$

$= U^* a_p U$ for some unitary map U on $\mathcal{F}(\{u_0\}^\perp)$
– the Bogoliubov transformation

We can think of b_p^*, b_p as new creation and annihilation operators. They satisfy the canonical commutation relations:
$[b_p, b_q] = 0$, $[b_p^*, b_q^*] = 0$, $[b_p, b_q^*] = \delta(p-q)$.

We have

$$\mathbb{H} \approx C_N + \mathbb{H}_{Bog}$$

$$= C_N + \frac{1}{2}\underbrace{\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \left(\sqrt{A_p^2 - B_p^2} - A_p\right)}_{=:\tilde{C}_N} + \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \underbrace{\sqrt{A_p^2-B_p^2}}_{=:e_p>0}\, b_p^* b_p$$

$$\underset{\substack{\uparrow\\ b_p = U^* a_p U \\ b_p^* = U^* a_p^* U}}{=} \tilde{C}_N + U^*\left(\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} e_p\, a_p^* a_p\right) U$$

The ground state of this operater is given by $\Psi_0 := U^* \underbrace{\Omega}_{\text{vacuum}}$.
Of course, Ψ_0 is only an approximation of the real ground state of H.

Recall that we would like to compute

$$\frac{1}{N}\left\langle \Psi_0, \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} a_p^* a_p \Psi_0\right\rangle = \frac{1}{N}\left\langle U^*\Omega, \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} a_p^* a_p U^*\Omega\right\rangle$$

$$= \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \|a_p U^*\Omega\|^2$$

<u>Claim</u>: $\|a_p U^*\Omega\|^2 + \|a_{-p} U^*\Omega\|^2 = 2\nu_p^2$

<u>Proof of the claim</u>:

Recall: $b_p = U^* a_p U = \sqrt{1+\nu_p^2}\, a_p + \nu_p a_{-p}^*$ and $\nu_p = \nu_{-p}$

We get $a_p = \frac{1}{\sqrt{1+\nu_p^2}} U^* a_p U - \frac{\nu_p}{\sqrt{1+\nu_p^2}} a_{-p}^*$ and therefore,

$$a_p U^*\Omega = \frac{1}{\sqrt{1+\nu_p^2}} \underbrace{U^* a_p \underbrace{U U^*}_{=\mathbb{1}}\Omega}_{=0} - \frac{\nu_p}{\sqrt{1+\nu_p^2}} a_{-p}^* U^*\Omega = \frac{-\nu_p}{\sqrt{1+\nu_p^2}} a_{-p}^* U^*\Omega$$

Thus,

$$\|a_p U^*\Omega\|^2 - \frac{\nu_p^2}{1+\nu_p^2}\underbrace{\|a_{-p}^* U^*\Omega\|^2}_{\langle U^*\Omega,\ \underbrace{a_{-p}a_{-p}^*}_{\substack{=[a_{-p},a_{-p}^*]+a_{-p}^*a_{-p} \\ =1 \quad + a_{-p}^*a_{-p}}} U^*\Omega\rangle} = \frac{\nu_p^2}{1+\nu_p^2} + \frac{\nu_p^2}{1+\nu_p^2}\|a_{-p} U^*\Omega\|^2$$

Similarly,

$$\|a_{-p} U^*\Omega\|^2 = \frac{\nu_p^2}{1+\nu_p^2} + \frac{\nu_p^2}{1+\nu_p^2}\|a_{+p} U^*\Omega\|^2.$$

If we add this equalities up, we obtain

$$\frac{1+\nu_p^2}{1+\nu_p^2}\left(\|a_p U^*\Omega\|^2 + \|a_{-p}U^*\Omega\|^2\right) - 2\frac{\nu_p^2}{1+\nu_p^2} + \frac{\nu_p^2}{1+\nu_p^2}\left(\|a_p U^*\Omega\|^2 + \|a_{-p}U^*\Omega\|^2\right).$$

It follows that

$$\|a_p U^*\Omega\|^2 + \|a_{-p}U^*\Omega\|^2 = 2\nu_p^2,$$

which proves the claim.

Hence,

$$\frac{1}{N}\langle\Psi_0, \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} a_p^* a_p \Psi_0\rangle = \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}}\|a_p U^*\Omega\|^2 \overset{\substack{\text{claim}\\ \downarrow}}{=} \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}}\nu_p^2$$

$$\underset{\substack{\uparrow \\ \text{def of} \\ \nu_p}}{=} \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}}\frac{1}{2}\left(\frac{A_p}{\sqrt{A_p^2-B_p^2}}-1\right) = \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}}\frac{A_p-\sqrt{A_p^2-B_p^2}}{2\sqrt{A_p^2-B_p^2}}$$

$$\underset{\substack{\uparrow \\ A_p=\frac{1}{L^2}|p|^2+N\hat{w}_L(p) \\ B_p=N\hat{w}_L(p)}}{=} \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}}\frac{\frac{1}{L^2}|p|^2+N\hat{w}_L(p)-\sqrt{\frac{1}{L^4}|p|^4+2\frac{1}{L^2}|p|^2N\hat{w}_L(p)}}{2\sqrt{\frac{1}{L^4}|p|^4+2\frac{1}{L^2}|p|^2N\hat{w}_L(p)}}$$

Recall:

$$\hat{w}_L(p) = \int_{\Lambda_1} dz\, e^{-ipz} w(Lz) \overset{\substack{\text{at least for small } p\\ \downarrow}}{\approx} \int_{\Lambda_1} dz\, w(Lz) = \frac{1}{L^3}\int_{\Lambda_1} dz\, L^3 w(Lz) = \frac{1}{L^3}\int_{\Lambda_L} dz\, w(z)$$

$$\underset{\substack{\uparrow \\ \text{for } L \text{ large enough}}}{=} \frac{1}{L^3}\int_{\mathbb{R}^3} dz\, w(z) \underset{\substack{\uparrow \\ \int w \approx 8\pi a}}{\approx} \frac{1}{L^3}8\pi a$$

Note: Actually, $\int w > 8\pi a$

Using this approximation, we get

$$\frac{1}{N}\langle \Psi_0, \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} a_p^* a_p \Psi_0\rangle$$

$$\approx \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \frac{\frac{1}{L^2}|p|^2 + N\frac{1}{L^3}8\pi a - \sqrt{\frac{1}{L^4}|p|^4 + 2\frac{1}{L^2}|p|^2 N\frac{1}{L^3}8\pi a}}{2\sqrt{\frac{1}{L^4}|p|^4 + 2\frac{1}{L^2}|p|^2 N\frac{1}{L^3}8\pi a}}$$

$$= \frac{1}{N}\sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \frac{|p|^2 + \frac{N}{L}8\pi a - \sqrt{|p|^4 + 2|p|^2\frac{N}{L}8\pi a}}{2\sqrt{|p|^4 + 2|p|^2\frac{N}{L}8\pi a}}$$

$$= \frac{1}{N} I\left(\frac{N}{L}8\pi a\right),$$

where $$I(b) := \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} \frac{|p|^2 + b - \sqrt{|p|^4 + 2|p|^2 b}}{2\sqrt{|p|^4 + 2|p|^2 b}}$$

We are working in the thermodynamic limit, i.e. $N\to\infty$, $L\to\infty$, $\frac{N}{L^3} = \rho$ fixed.
In particular, $b = \frac{N}{L}8\pi a \longrightarrow \infty$. Now

$$I(b) = \sum_{z=\frac{p}{\sqrt{b}}} \frac{|z|^2 + 1 - \sqrt{|z|^4 + 2|z|^2}}{2\sqrt{|z|^4 + 2|z|^2}}$$

for $p\in 2\pi\mathbb{Z}^3\setminus\{0\}$

$$\underset{\text{Riemann integral}}{\overset{\text{for large } b}{\approx}} \frac{1}{\left(\frac{2\pi}{\sqrt{b}}\right)^3}\int_{\mathbb{R}^3} dz\, \frac{|z|^2 + 1 - \sqrt{|z|^4 + 2|z|^2}}{2\sqrt{|z|^4 + 2|z|^2}}$$

$$\overset{\text{polar coord.}}{=} \sqrt{b^3}\,\underbrace{\frac{1}{(2\pi)^3}4\pi}_{=\frac{1}{2\pi^2}}\ \underbrace{\int_0^\infty dr\, r^2\,\frac{r^2+1-\sqrt{r^4+2r^2}}{2\sqrt{r^4+2r^2}}}_{=\frac{1}{3\sqrt{2}}}$$

Mathematica

$$= \frac{1}{6\sqrt{2}\,\pi^2}\sqrt{b^3}$$

It follows that

$$I\left(\frac{N}{L}8\pi a\right) \simeq \frac{1}{6\sqrt{2}\,\pi^2}\sqrt{\left(\frac{N}{L}8\pi a\right)^3} = \frac{8\sqrt{8}}{6\sqrt{2}}\frac{1}{\sqrt{\pi}}\sqrt{\frac{N^3}{L^3}}\sqrt{a^3}$$

$$= \frac{4\sqrt{4}}{3}\frac{1}{\sqrt{\pi}}\sqrt{\frac{N}{L^3}}\,N\sqrt{a^3} \underset{\varrho = \frac{N}{L^3}}{\overset{\uparrow}{=}} N\frac{8}{3\sqrt{\pi}}\sqrt{\varrho}\sqrt{a^3}.$$

We get

$$\frac{1}{N}\left\langle \Psi_0, \sum_{p\in 2\pi\mathbb{Z}^3\setminus\{0\}} a_p^* a_p \Psi_0\right\rangle \simeq \frac{1}{N} I\left(\frac{N}{L}8\pi a\right) = \underline{\underline{\frac{8}{3\sqrt{\pi}}\sqrt{\varrho a^3}}},$$

which is also the result for η as $\varrho \to 0$ in the paper on the simple equation.