Excitation spectrum of interacting bosons in the mean field infinite volume limit

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We would like to show that in a certain limit low lying excitation spectrum of an N-body Schrödinger Hamiltonian with repulsive interaction is given by the Bogoliubov approximation. This limit will involve $N \to \infty$, weak coupling and large density. It will allow for an arbitrarily large size of the box provided that it does not grow too fast.

Potential

We start with a real function v on $\mathbb{R}^d$. We assume that $v(\mathrm{x}) = v(-\mathrm{x})$ and that

$$v \in L^1(\mathbb{R}^d), \quad \hat{v} \in L^1(\mathbb{R}^d),$$

$$v(\mathrm{x}) \geq 0, \quad \mathrm{x} \in \mathbb{R}^d, \qquad \hat{v}(\mathrm{p}) \geq 0, \quad \mathrm{p} \in \mathbb{R}^d.$$

Then we replace the infinite space $\mathbb{R}^d$ by the torus $]-L/2, L/2]^d$. The potential v is replaced by its periodized version

$$v^L(\mathrm{x}) = \frac{1}{(2\pi L)^d} \sum_{\mathrm{p} \in (2\pi/L)\mathbb{Z}^d} \mathrm{e}^{\mathrm{ipx}} \hat{v}(\mathrm{p}).$$

We will always assume that $L \geq 1$.

Hamiltonian

$$H_N^L = -\sum_{i=1}^{N} \Delta_i^L + \frac{L^d}{N} \sum_{1\le i<j\le N} v^L(\mathrm{x}_i - \mathrm{x}_j). \tag{0.1}$$

Total momentum

$$P_N^L := -\sum_{i=1}^{N} \mathrm{i}\partial_{\mathrm{x}_i}^L. \tag{0.2}$$

From now on, we will drop the superscripts L.

We will denote by E_N the ground state energy of H_N.

For $\mathrm{p} \in \frac{2\pi}{L}\mathbb{Z}^d \backslash \{0\}$, let $K_N^1(\mathrm{p}), K_N^2(\mathrm{p}), \dots$ be the corresponding excitation energies, that is, the eigenvalues of $H_N - E_N$ of total momentum p in the increasing order.

The lowest eigenvalue of $H_N - E_N$ of total momentum $\mathrm{p} = 0$ is 0 by general arguments. Let $K_N^1(0), K_N^2(0), \dots$ be the next eigenvalues of $H_N - E_N$ of total momentum 0, also in the increasing order.

Introduce the Bogoliubov energy

$$E_{\mathrm{Bog}} := -\frac{1}{2} \sum_{\mathrm{p} \in \frac{2\pi}{L}\mathbb{Z}^d \setminus \{0\}} \left(|\mathrm{p}|^2 + \hat{v}(\mathrm{p}) - \sqrt{|\mathrm{p}|^4 + 2\hat{v}(\mathrm{p})|\mathrm{p}|^2} \right).$$

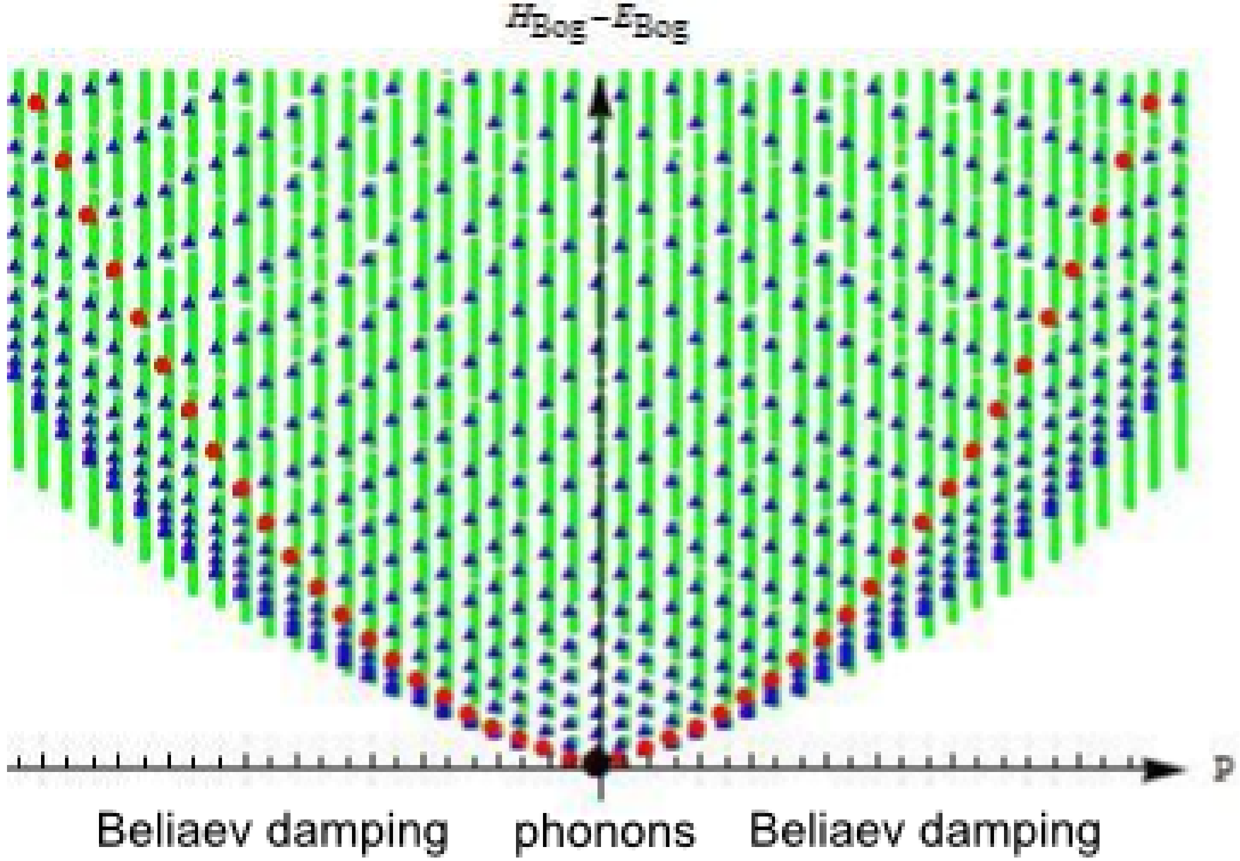
and the Bogoliubov elementary excitation spectrum

$$e_{\mathrm{p}} = \sqrt{|\mathrm{p}|^4 + 2\hat{v}(\mathrm{p})|\mathrm{p}|^2}, \tag{0.3}$$

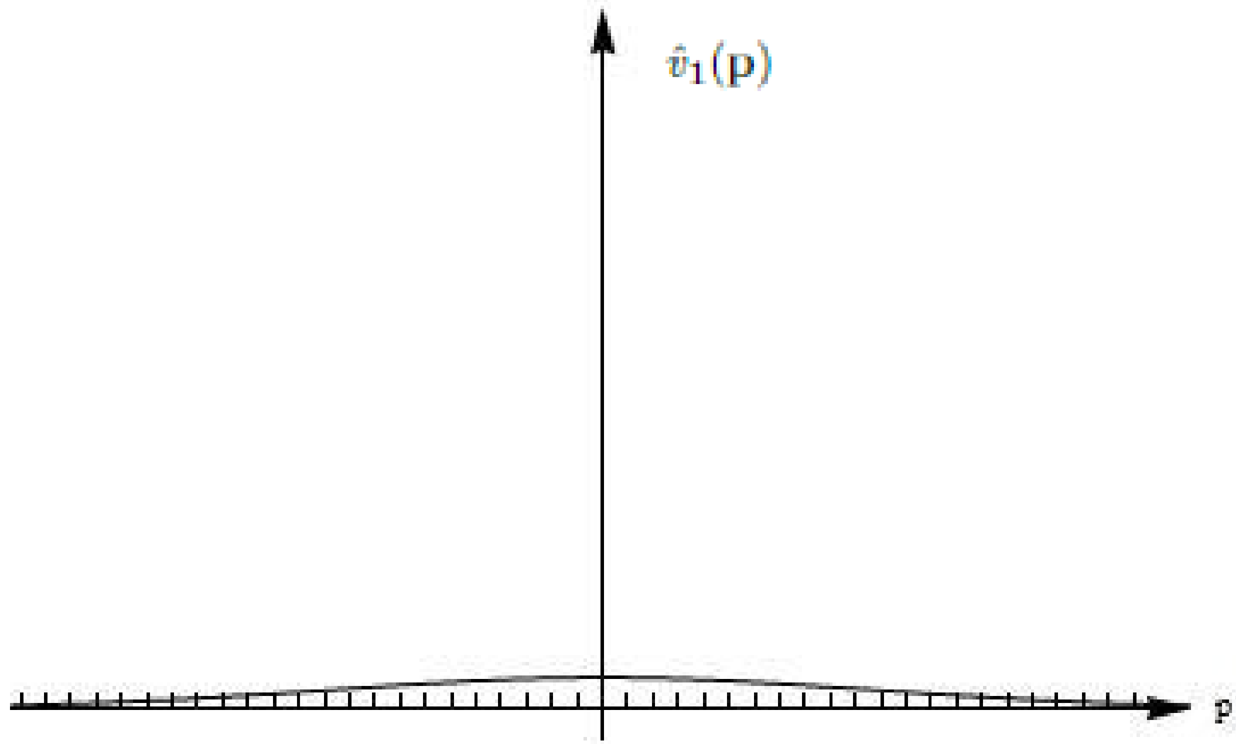
For any $\mathrm{p} \in \frac{2\pi}{L}\mathbb{Z}^d$ we consider the Bogoliubov excitation energies with total momentum p:

$$\Big\{ \sum_{i=1}^{j} e_{\mathrm{k}_i} \ : \ \mathrm{k}_1, \dots, \mathrm{k}_j \in \frac{2\pi}{L}\mathbb{Z}^d, \ \mathrm{k}_1 + \cdots + \mathrm{k}_j = \mathrm{p}, \quad j = 1, 2, \dots \Big\}.$$

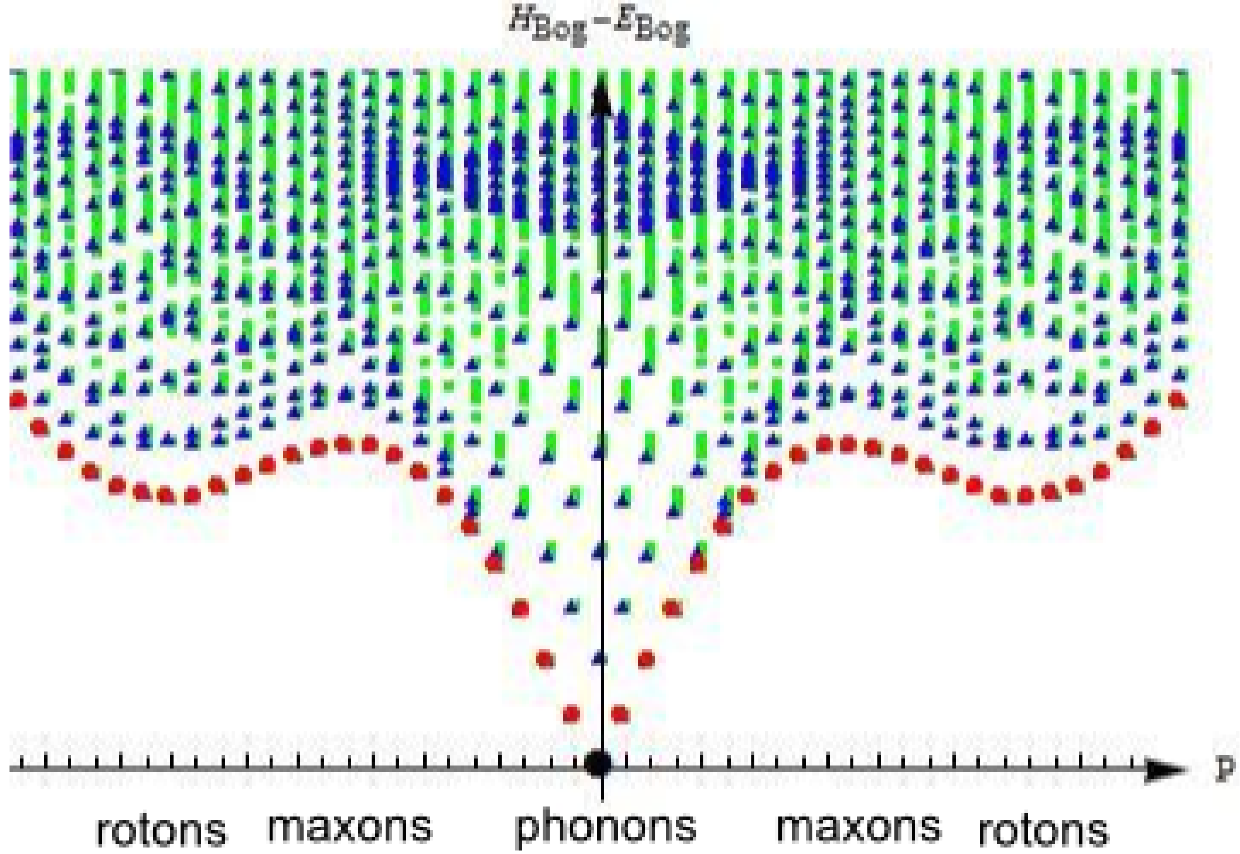
Let $K^1_{\mathrm{Bog}}(\mathrm{p}), K^2_{\mathrm{Bog}}(\mathrm{p}), \dots$ be these excitation energies in the increasing order.



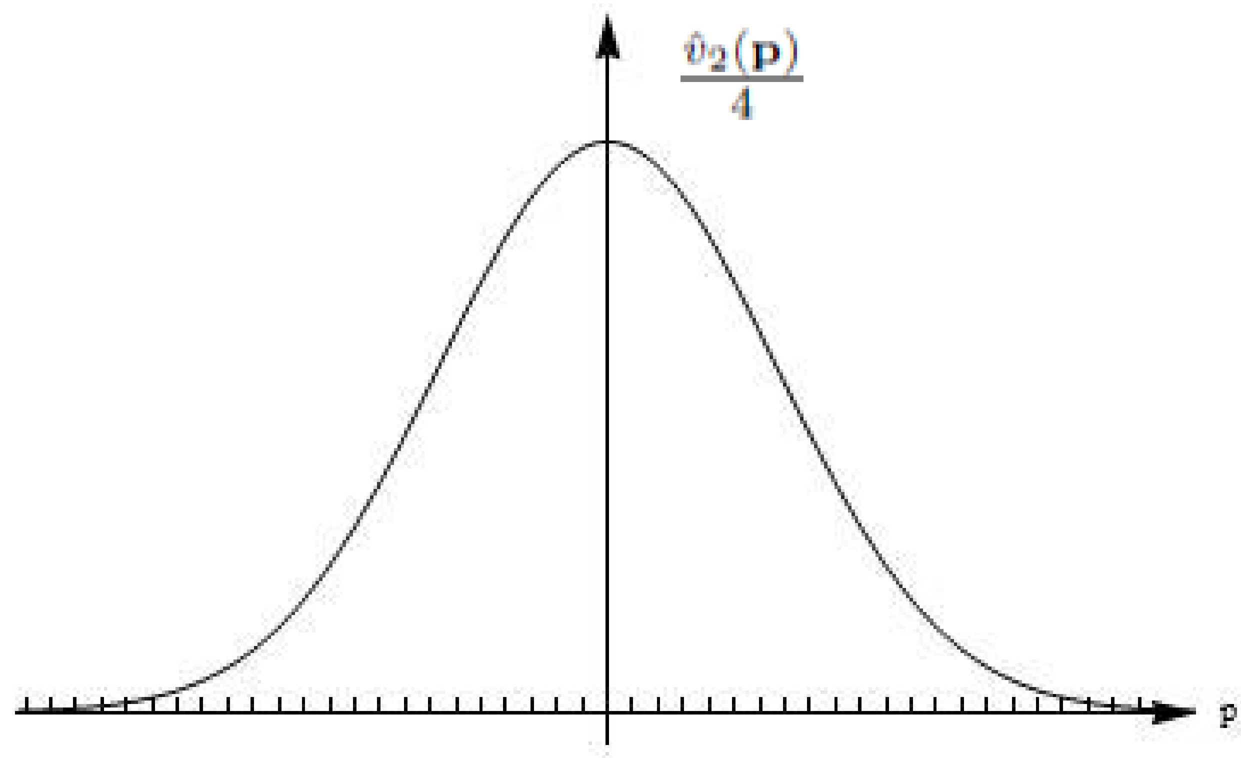
$H_{Bog} - E_{Bog}$
p
Beliaev damping
phonons
Beliaev damping



$$\hat{v}_1(\mathrm{p}) = \frac{\mathrm{e}^{-\mathrm{p}^2/5}}{10}.$$



$H_{Bog} - E_{Bog}$
p
rotons
maxons
phonons
maxons
rotons


$\frac{\hat{v}_2(\mathbf{p})}{4}$
p

Lower bound.

Suppose that $L^{2d+2} \leq N$. Then there exists C such that

$$E_N \geq \frac{1}{2}\hat{v}(0)(N-1) + E_{\text{Bog}} - CN^{-1/2}L^{2d+3}.$$

Moreover, if $\kappa \geq 0$ and $L^{d+2}(L^d + \kappa) \leq N$ then there exists C such that if $K_N^j(\mathrm{p}) \leq \kappa$, then

$$\begin{aligned} E_N + K_N^j(\mathrm{p}) \;\geq\; & \frac{1}{2}\hat{v}(0)(N-1) + E_{\text{Bog}} + K_{\text{Bog}}^j(\mathrm{p}) \\ & -CN^{-1/2}L^{d/2+3}(\kappa + L^d)^{3/2}. \end{aligned}$$

Upper bound.

Suppose that $L^{2d+1} \leq N$. Then then there exists C such that

$$E_N \leq \frac{1}{2}\hat{v}(0)(N-1) + E_{\mathrm{Bog}} + CN^{-1/2}L^{2d+3/2}.$$

Moreover, if $\kappa \geq 0$ and $L^{d+2}(\kappa + L^{d-1}) \leq N$, then there exists C such that if $K^j_{\mathrm{Bog}}(\mathrm{p}) \leq \kappa$, then

$$\begin{aligned} E_N + K^j_N(\mathrm{p}) \;&\leq\; \frac{1}{2}\hat{v}(0)(N-1) + E_{\mathrm{Bog}} + K^j_{\mathrm{Bog}}(\mathrm{p}) \\ &\quad + CN^{-1/2}L^{d/2+3}(\kappa + L^{d-1})^{3/2}. \end{aligned}$$

Special case of this theorem with $L = 1$ was proven by R. Seiringer.

Mimicking his proof gives big error terms – they are of the order $N^{-1/2}\exp(L^{d/2})$. To get better error estimates we need to modify somewhat his method.

Consequences of the min-max principle

Let A be a bounded from below self-adjoint operator with discrete spectrum. We define

$$\overrightarrow{\mathrm{sp}}(A) := (E_1, E_2, \dots),$$

where $E_1, E_2, \dots$ are the eigenvalues of A in the increasing order. If $\dim \mathcal{H} = n$, then we set $E_{n+1} = E_{n+2} = \cdots = \infty$.

$$A \le B \text{ implies } \overrightarrow{\mathrm{sp}}(A) \le \overrightarrow{\mathrm{sp}}(B).$$

Rayleigh-Ritz principle

$$\overrightarrow{\mathrm{sp}}(A) \le \overrightarrow{\mathrm{sp}}\Big(P_{\mathcal{K}} A P_{\mathcal{K}}\Big|_{\mathcal{K}}\Big). \tag{0.4}$$

Fock space

$$\mathcal{H} := \bigoplus_{N=0}^{\infty} \mathcal{H}_N = \Gamma_{\mathrm{s}}\Big(l^2\big(\frac{2\pi}{L}\mathbb{Z}^d\big)\Big).$$

Second quantization notation

$$H := \bigoplus_{N=0}^{\infty} H_N = \sum_{\mathrm{p}} \mathrm{p}^2 a_{\mathrm{p}}^\dagger a_{\mathrm{p}} + \frac{1}{2N} \sum_{\mathrm{p,q,k}} \hat{v}(\mathrm{k}) a_{\mathrm{p+k}}^\dagger a_{\mathrm{q-k}}^\dagger a_{\mathrm{q}} a_{\mathrm{p}}.$$

Number of particles in and outside of the condensate

$$N_0 = a_0^\dagger a_0, \quad N^> = \sum_{\mathrm{p}\neq 0} a_{\mathrm{p}}^\dagger a_{\mathrm{p}}.$$

Estimating Hamiltonian

$$
\begin{aligned}
H_\epsilon \;:=\; & \frac{1}{2}\hat{v}(0)(N-1) + \sum_{\mathrm{p}\neq 0}\big(|\mathrm{p}|^2 + \hat{v}(\mathrm{p})\big)a_{\mathrm{p}}^\dagger a_{\mathrm{p}} \\
& + \frac{1}{2}\sum_{\mathrm{p}\neq 0}\hat{v}(\mathrm{p})\Big(\frac{a_0^\dagger a_0^\dagger}{N}a_{\mathrm{p}}a_{-\mathrm{p}} + a_{\mathrm{p}}^\dagger a_{-\mathrm{p}}^\dagger\frac{a_0 a_0}{N}\Big) \\
& - \frac{1}{N}\sum_{\mathrm{p}\neq 0}\big(\hat{v}(\mathrm{p}) + \frac{\hat{v}(0)}{2}\big)a_{\mathrm{p}}^\dagger a_{\mathrm{p}} N^{>} + \frac{\hat{v}(0)}{2N}N^{>} \\
& + \frac{\epsilon}{N}\sum_{\mathrm{p}\neq 0}\big(\hat{v}(\mathrm{p}) + \hat{v}(0)\big)a_{\mathrm{p}}^\dagger a_{\mathrm{p}} N_0 \\
& + (1+\epsilon^{-1})\frac{1}{2N}v(0)L^d N^{>}(N^{>}-1).
\end{aligned}
$$

$$
H \;\geq\; H_{-\epsilon}, \quad 0 < \epsilon \leq 1; \tag{0.5}
$$

$$
H \;\leq\; H_{\epsilon}, \quad 0 < \epsilon. \tag{0.6}
$$

The exponential property of Fock spaces gives

$$\mathcal{H} \simeq \Gamma_{\mathrm{s}}(\mathbb{C}) \otimes \Gamma_{\mathrm{s}}\Big(l^2\big(\frac{2\pi}{L}\mathbb{Z}^d\backslash\{0\}\big)\Big). \tag{0.7}$$

Embed the space of the zeroth mode $\Gamma_{\mathrm{s}}(\mathbb{C}) = l^2(\{0,1,\dots\})$ in a larger space $l^2(\mathbb{Z})$. Thus we obtain the extended space

$$\mathcal{H}^{\mathrm{ext}} := l^2(\mathbb{Z}) \otimes \Gamma_{\mathrm{s}}\Big(l^2\big(\frac{2\pi}{L}\mathbb{Z}^d\backslash\{0\}\big)\Big). \tag{0.8}$$

The operator N_0 extends to an operator N_0^{ext} and

$$\mathcal{H} = \mathrm{Ran}\mathbb{1}_{[0,\infty[}(N_0^{\mathrm{ext}}).$$

For $N \in \mathbb{Z}$, we will write $\mathcal{H}_N^{\mathrm{ext}}$ for the subspace of $\mathcal{H}^{\mathrm{ext}}$ corresponding to $N^> + N_0^{\mathrm{ext}} = N$.

We have also a unitary operator

$$U|n_0\rangle \otimes \Psi^{>} = |n_0 - 1\rangle \otimes \Psi^{>}.$$

We define for $\mathrm{p} \neq 0$ the following operator on $\mathcal{H}^{\mathrm{ext}}$:

$$b_{\mathrm{p}} := a_{\mathrm{p}} U^{\dagger}.$$

b_{p} and $b_{\mathrm{q}}^{\dagger}$ satisfy the same CCR as a_{p} and $a_{\mathrm{q}}^{\dagger}$.

Extended estimating Hamiltonian.

$$\begin{aligned}
H_{N,\epsilon}^{\text{ext}} \;:=\; & \frac{1}{2}\hat{v}(0)(N-1)+\sum_{\mathrm{p}\neq 0}\big(|\mathrm{p}|^2+\hat{v}(\mathrm{p})\big)b_{\mathrm{p}}^{\dagger}b_{\mathrm{p}} \\
& +\frac{1}{2}\sum_{\mathrm{p}\neq 0}\hat{v}(\mathrm{p})\Big(\frac{\sqrt{(N_0^{\text{ext}}-1)N_0^{\text{ext}}}}{N}b_{\mathrm{p}}b_{-\mathrm{p}}+\mathrm{hc}\Big) \\
& -\frac{1}{N}\sum_{\mathrm{p}\neq 0}\big(\hat{v}(\mathrm{p})+\frac{\hat{v}(0)}{2}\big)b_{\mathrm{p}}^{\dagger}b_{\mathrm{p}}N^{>}+\frac{\hat{v}(0)}{2N}N^{>} \\
& +\frac{\epsilon}{N}\sum_{\mathrm{p}\neq 0}\big(\hat{v}(\mathrm{p})+\hat{v}(0)\big)b_{\mathrm{p}}^{\dagger}b_{\mathrm{p}}N_0^{\text{ext}} \\
& +(1+\epsilon^{-1})\frac{1}{2N}v(0)L^{d}N^{>}(N^{>}-1).
\end{aligned}$$

$H_{N,\epsilon}^{\text{ext}}$ acts on $\mathcal{H}_N^{\text{ext}}$. It preserves the physical N-particle space $\mathcal{H}_N$ and restricted to it coincides with $H_{N,\epsilon}$.

The operator

$$\sum_{\mathrm{p}\neq 0}\big(|\mathrm{p}|^2+\hat{v}(\mathrm{p})\big)b_{\mathrm{p}}^\dagger b_{\mathrm{p}}+\frac{1}{2}\sum_{\mathrm{p}\neq 0}\hat{v}(\mathrm{p})\Big(b_{\mathrm{p}}b_{-\mathrm{p}}+b_{\mathrm{p}}^\dagger b_{-\mathrm{p}}^\dagger\Big).$$

preserves $\mathcal{H}_N^{\mathrm{ext}}$. Its restriction to $\mathcal{H}_N^{\mathrm{ext}}$ will be denoted $H_{\mathrm{Bog},N}$.

We can write

$$\begin{aligned}
H_{N,\epsilon}^{\mathrm{ext}} &= \frac{1}{2}\hat{v}(0)(N-1)+H_{\mathrm{Bog},N}+R_{N,\epsilon}, &(0.9)\\
R_{N,\epsilon} &:= \frac{1}{2}\sum_{\mathrm{p}\neq 0}\hat{v}(\mathrm{p})\Big(\Big(\frac{\sqrt{(N_0^{\mathrm{ext}}-1)N_0^{\mathrm{ext}}}}{N}-1\Big)b_{\mathrm{p}}b_{-\mathrm{p}}+\mathrm{hc}\Big)\\
&\quad -\frac{1}{N}\sum_{\mathrm{p}\neq 0}\big(\hat{v}(\mathrm{p})+\frac{\hat{v}(0)}{2}\big)b_{\mathrm{p}}^\dagger \mathrm{b}_{\mathrm{p}}N^{>}+\frac{\hat{v}(0)}{2N}N^{>}\\
&\quad +\frac{\epsilon}{N}\sum_{\mathrm{p}\neq 0}\big(\hat{v}(\mathrm{p})+\hat{v}(0)\big)b_{\mathrm{p}}^\dagger b_{\mathrm{p}}N_0^{\mathrm{ext}}\\
&\quad +(1+\epsilon^{-1})\frac{1}{2N}v(0)L^dN^{>}(N^{>}-1). &(0.10)
\end{aligned}$$

$H_{\mathrm{Bog},N}$ are unitarily equivalent to one another for every N. They are equivalent to

$$E_{\mathrm{Bog}} + \sum_{\mathrm{p}\neq 0} e_{\mathrm{p}} a_{\mathrm{p}}^{\dagger} a_{\mathrm{p}},$$

where

$$\begin{aligned} E_{\mathrm{Bog}} &:= -\frac{1}{2} \sum_{\mathrm{p}\in\frac{2\pi}{L}\mathbb{Z}^d\setminus\{0\}} \left(|\mathrm{p}|^2 + \hat{v}(\mathrm{p}) - \sqrt{|\mathrm{p}|^4 + 2\hat{v}(\mathrm{p})|\mathrm{p}|^2} \right), \\ e_{\mathrm{p}} &:= \sqrt{|\mathrm{p}|^4 + 2\hat{v}(\mathrm{p})|\mathrm{p}|^2}. \end{aligned}$$

Proof of lower bound

For brevity, set

$$\mathbb{1}_\kappa^N := \mathbb{1}_{[0,\kappa]}(H_N - E_N).$$

For $0 < \epsilon \leq 1$

$$\mathbb{1}_\kappa^N H_N \mathbb{1}_\kappa^N \geq \mathbb{1}_\kappa^N \left(\frac{1}{2}\hat{v}(0)(N-1) + H_{\mathrm{Bog},N} + R_{N,-\epsilon} \right) \mathbb{1}_\kappa^N$$

Hence

$$\overrightarrow{\mathrm{sp}}\big(\mathbb{1}_\kappa^N H_N \mathbb{1}_\kappa^N\big) \geq \frac{1}{2}\hat{v}(0)(N-1) + \overrightarrow{\mathrm{sp}}\big(H_{\mathrm{Bog}}\big) - \big\|\mathbb{1}_\kappa^N R_{N,-\epsilon} \mathbb{1}_\kappa^N\big\|.$$

Proof of upper bound

Suppose that G is a smooth nonnegative function on $[0,\infty[$ such that

$$G(s) = \begin{cases} 1, & \text{if } s \in [0, \frac{1}{3}] \\ 0, & \text{if } s \in [1, \infty[. \end{cases} \tag{0.11}$$

For brevity, set

$$\mathbb{1}_\kappa^{\text{Bog}} := \mathbb{1}_{[0,\kappa]}(H_{\text{Bog},N} - E_{\text{Bog}}).$$

We define

$$Z_\kappa := \big(\mathbb{1}_\kappa^{\text{Bog}} G(N^>/N)^2 \mathbb{1}_\kappa^{\text{Bog}}\big)^{-1/2} \mathbb{1}_\kappa^{\text{Bog}} G(N^>/N).$$

Clearly, Z_κ is a partial isometry with initial space $\text{Ran}(A_N \mathbb{1}_\kappa^{\text{Bog}})$ and final space $\text{Ran}(\mathbb{1}_\kappa^{\text{Bog}})$.

$$\overrightarrow{\mathrm{sp}} H_N \;\le\; \overrightarrow{\mathrm{sp}}\left(Z_\kappa^\dagger Z_\kappa H_N Z_\kappa^\dagger Z_\kappa \Big|_{\mathrm{Ran} Z_\kappa^\dagger} \right) \;=\; \overrightarrow{\mathrm{sp}}\left(Z_\kappa H_N Z_\kappa^\dagger \Big|_{\mathrm{Ran} \mathbb{1}_\kappa^{\mathrm{Bog}}} \right).$$

Moreover,

$$\begin{aligned} Z_\kappa H_N Z_\kappa^\dagger &\le Z_\kappa H_{N,\epsilon} Z_\kappa^\dagger \\ &= \frac{1}{2}\hat{v}(0)(N-1)\mathbb{1}_\kappa^{\mathrm{Bog}} + H_{\mathrm{Bog}}\mathbb{1}_\kappa^{\mathrm{Bog}} \\ &\quad + Z_\kappa(H_{\mathrm{Bog}} - E_{\mathrm{Bog}})Z_\kappa^\dagger - (H_{\mathrm{Bog}} - E_{\mathrm{Bog}})\mathbb{1}_\kappa^{\mathrm{Bog}} \\ &\quad + Z_\kappa R_{N,\epsilon} Z_\kappa^\dagger. \end{aligned}$$

Hence,

$$\begin{aligned} \overrightarrow{\mathrm{sp}} H_N &\le \frac{1}{2}\hat{v}(0)(N-1) + \overrightarrow{\mathrm{sp}}\left(\mathbb{1}_\kappa^{\mathrm{Bog}} H_{\mathrm{Bog}} \mathbb{1}_\kappa^{\mathrm{Bog}} \right) \\ &\quad + \left\| Z_\kappa(H_{\mathrm{Bog}} - E_{\mathrm{Bog}})Z_\kappa^\dagger - (H_{\mathrm{Bog}} - E_{\mathrm{Bog}})\mathbb{1}_\kappa^{\mathrm{Bog}} \right\| \\ &\quad + \left\| Z_\kappa R_{N,\epsilon} Z_\kappa^\dagger \right\|. \end{aligned}$$