

Excitation Spectra of Bose-Einstein Condensates

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Recent Results on Quantum Many-Body Systems
Herrsching

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Hamilton operator: N bosons in $\Lambda = [0; 1]^3$ described by

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \kappa \sum_{i < j}^N N^2 V(N(x_i - x_j)), \quad \text{on } L_s^2(\Lambda^N)$$

$\kappa > 0$ is coupling constant, $V \geq 0$ short range interaction.

Scattering length: defined by zero-energy **scattering equation**

$$\left[-\Delta + \frac{\kappa}{2} V \right] f = 0, \quad \text{with} \quad f(x) \rightarrow 1 \quad \text{as } |x| \rightarrow \infty$$

$$\Rightarrow \quad f(x) = 1 - \frac{a_0}{|x|}, \quad \text{for large } |x|$$

Here a_0 is scattering length of V . Equivalently,

$$8\pi a_0 = \kappa \int V(x) f(x) dx$$

By **scaling**, $\kappa N^2 V(N \cdot)$ has scattering length a_0/N .

Ground state energy: from [Lieb-Yngvason '98], ground state energy given to leading order by

$$E_N = 4\pi a_0 N + o(N)$$

Bose-Einstein condensation: from [Lieb-Seiringer '02], ground state ψ_N exhibits BEC, i.e. $\gamma_N = \text{Tr}_{2,\dots,N} |\psi_N\rangle\langle\psi_N|$ is such that

$$\gamma_N \rightarrow |\varphi_0\rangle\langle\varphi_0|$$

with $\varphi_0(x) = 1$ for all $x \in \Lambda$.

Warning: this does not mean that $\psi_N \simeq \varphi_0^{\otimes N}$. A simple computation shows

$$\langle \varphi_0^{\otimes N}, H_N \varphi_0^{\otimes N} \rangle = \frac{(N-1)}{2} \kappa \hat{V}(0) \gg 4\pi a_0 N$$

Correlations play crucial role!!

Theorem [BBCS, '18]: Suppose $\kappa > 0$ is **small enough**. Then

$$E_N = 4\pi\mathfrak{a}_N(N-1) - \frac{1}{2} \sum_{p \in \Lambda_+^*} \left[p^2 + 8\pi\mathfrak{a}_0 - \sqrt{|p|^4 + 16\pi\mathfrak{a}_0 p^2} - \frac{(8\pi\mathfrak{a}_0)^2}{2p^2} \right] + \mathcal{O}(N^{-1/4})$$

where $\Lambda_+^* = 2\pi\mathbb{Z}^3 \setminus \{0\}$ and

$$8\pi\mathfrak{a}_N = \kappa \hat{V}(0) + \sum_{k=1}^{\infty} \frac{(-1)^k \kappa^{k+1}}{(2N)^k} \times \sum_{p_1, \dots, p_k \in \Lambda_+^*} \frac{\hat{V}(p_1/N)}{p_1^2} \left(\prod_{i=1}^{k-1} \frac{\hat{V}((p_i - p_{i+1})/N)}{p_{i+1}^2} \right) \hat{V}(p_k/N)$$

Moreover, **spectrum** of $H_N - E_N$ below ζ consists of eigenvalues

$$\sum_{p \in \Lambda_+^*} n_p \sqrt{|p|^4 + 16\pi\mathfrak{a}_0 p^2} + \mathcal{O}(N^{-1/4}(1 + \zeta^3))$$

where $n_p \in \mathbb{N}$ for all $p \in \Lambda_+^*$.

Remark 1: definition of \mathfrak{a}_N can be compared with **Born series**

$$8\pi\mathfrak{a}_0 = \kappa\hat{V}(0) + \sum_{k=1}^{\infty} \frac{(-1)^k \kappa^{k+1}}{2^k (2\pi)^{3k}} \\ \times \int_{\mathbb{R}^{3k}} dp_1 \dots dp_k \frac{\hat{V}(p_1)}{p_1^2} \left(\prod_{i=1}^{k-1} \frac{\hat{V}(p_i - p_{i+1})}{p_{i+1}^2} \right) \hat{V}(p_k)$$

for \mathfrak{a}_0 . We find

$$|\mathfrak{a}_N - \mathfrak{a}_0| \leq CN^{-1}$$

At the level of precision of Theorem, ground state energy sensitive to **finite volume** effects!

Remark 2: Gross-Pitaevskii regime equivalent to N particles in box with volume N^3 interacting through unscaled potential V .

Thermodynamic limit: N particles in box Λ , with $N, |\Lambda| \rightarrow \infty$ and $\rho = N/|\Lambda|$ fixed.

Lee-Huang-Yang formula: for small ρ , ground state energy per particles expected to obey

$$\lim_{\substack{N, |\Lambda| \rightarrow \infty \\ \rho = N/|\Lambda|}} \frac{E_N}{N} = 4\pi a_0 \rho \left[1 + \frac{128}{15\sqrt{\pi}} (\rho a_0^3)^{1/2} + \dots \right]$$

Rigorous results: [Dyson, '58], [Lieb-Yngvason, '98], [Erdős-S.-Yau, '08], [Yau-Yin, '09], [Giuliani-Seiringer, '09], [Brietzke-Solovej, '18] (extending ideas from [Lieb-Solovej, '01]).

Previous works: mathematically simpler models described by

$$H_N^\beta = \sum_{j=1}^N -\Delta_{x_j} + \frac{\kappa}{N} \sum_{i < j}^N N^{3\beta} V(N^\beta(x_i - x_j))$$

for $\beta \in [0; 1)$.

In **mean field regime**, $\beta = 0$, excitation spectrum determined by [Seiringer, '11], [Grech-Seiringer, '13], [Lewin-Nam-Serfaty-Solovej, '14], [Derezinski-Napiorkowski, '14], [Pizzo, '16].

Dispersion of excitations given by $\varepsilon_{\text{mf}}(p) = \sqrt{|p|^4 + 2\kappa \hat{V}(p)p^2}$.

For **intermediate regimes**, $\beta \in (0; 1)$, excitations spectrum determined by [BBCS, '17].

Dispersion of excitations given by $\varepsilon_\beta(p) = \sqrt{|p|^4 + 2\kappa \hat{V}(0)p^2}$.

Bogoliubov approximation: rewrite H_N in momentum space, using second quantization:

$$H_N = \sum_{p \in \Lambda^*} p^2 a_p^* a_p + \frac{\kappa}{2N} \sum_{p, q, r \in \Lambda^*} \hat{V}(r/N) a_{p+r}^* a_q^* a_p a_{q+r}$$

where, a_p^*, a_p are **creation** and **annihilation operators** with

$$[a_p, a_q^*] = \delta_{pq}, \quad [a_p, a_q] = [a_p^*, a_q^*] = 0$$

BEC implies a_0, a_0^* are much larger than $[a_0, a_0^*] = 1$. Hence, Bogoliubov **replaced** all a_0, a_0^* by factors of \sqrt{N} .

In the resulting Hamiltonian, he **neglected** all contributions cubic and quartic in $a_p, a_p^*, p \neq 0$.

Then he **diagonalized** the quadratic Hamiltonian he derived.

Finally, he recognised that some expressions were first and second **Born approximations** for a_0 and he replaced them with a_0 .

Orthogonal excitations: for $\psi_N \in L_s^2(\Lambda^N)$ and $\varphi_0 \equiv 1$ on Λ , write

$$\psi_N = \alpha_0 \varphi_0^{\otimes N} + \alpha_1 \otimes_s \varphi_0^{\otimes(N-1)} + \alpha_2 \otimes_s \varphi_0^{\otimes(N-2)} + \dots + \alpha_N$$

where $\alpha_j \in L_{\perp\varphi_0}^2(\Lambda)^{\otimes_s j}$.

As in [Lewin-Nam-Serfaty-Solovej, '12], define **unitary map**

$$U : L_s^2(\Lambda^N) \rightarrow \mathcal{F}_+^{\leq N} := \bigoplus_{j=0}^N L_{\perp\varphi_0}^2(\Lambda)^{\otimes_s j}$$

$$\psi_N \rightarrow U\psi_N = \{\alpha_0, \alpha_1, \dots, \alpha_N\}$$

Excitation Hamiltonian: we use unitary map U to define

$$\mathcal{L}_N = UH_NU^* : \mathcal{F}_+^{\leq N} \rightarrow \mathcal{F}_+^{\leq N}$$

For $p, q \in \Lambda_+^* = 2\pi\mathbb{Z}^3 \setminus \{0\}$, we have

$$\begin{aligned} U a_p^* a_q U^* &= a_p^* a_q, & U a_0^* a_0 U^* &= N - \mathcal{N}_+ \\ U a_p^* a_0 U^* &= a_p^* \sqrt{N - \mathcal{N}_+}, & U a_0^* a_p U^* &= \sqrt{N - \mathcal{N}_+} a_p \end{aligned}$$

Hence, similarly to **Bogoliubov approximation**,

$$\begin{aligned} \mathcal{L}_N &= \frac{(N-1)}{2N} \kappa \hat{V}(0) (N - \mathcal{N}_+) + \frac{\kappa \hat{V}(0)}{2N} \mathcal{N}_+ (N - \mathcal{N}_+) \\ &\quad + \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p + \sum_{p \in \Lambda_+^*} \kappa \hat{V}(p/N) a_p^* \frac{N-1-\mathcal{N}_+}{N} a_p \\ &\quad + \frac{\kappa}{2} \sum_{p \in \Lambda_+^*} \hat{V}(p/N) \left[a_p^* a_{-p}^* \sqrt{\frac{(N-\mathcal{N}_+)(N-1-\mathcal{N}_+)}{N^2}} + \text{h.c.} \right] \\ &\quad + \frac{\kappa}{\sqrt{N}} \sum_{p, q \in \Lambda_+^* : p+q \neq 0} \hat{V}(p/N) \left[\sqrt{\frac{N+1-\mathcal{N}_+}{N}} a_{p+q}^* a_{-p}^* a_q + \text{h.c.} \right] \\ &\quad + \frac{\kappa}{2N} \sum_{p, q \in \Lambda_+^*, r \in \Lambda^* : r \neq -p, -q} \hat{V}(r/N) a_{p+r}^* a_q^* a_p a_{q+r} \end{aligned}$$

Gain: conjugation with U generates new **constant** and **quadratic** contributions.

Problem: in contrast with mean-field regime, after conjugation with U there are still **large contributions** in higher order terms.

Reason: $U^*\Omega = \varphi_0^{\otimes N}$ not good approximation for ground state!
We need to take into account **correlations**!

Natural idea: conjugate \mathcal{L}_N with a **Bogoliubov** transformation of the form

$$\tilde{T} = \exp \left[\frac{1}{2} \sum_{p \in \Lambda_+^*} \eta_p \left(a_p^* a_{-p}^* - a_p a_{-p} \right) \right]$$

so that

$$\tilde{T}^* a_p \tilde{T} = a_p \cosh(\eta_p) + a_{-p}^* \sinh(\eta_p)$$

Challenge: \tilde{T} does not preserve the excitation space $\mathcal{F}_+^{\leq N}$.

Modified operators: for $p \in \Lambda_+^*$, define

$$b_p^* = a_p^* \sqrt{\frac{N - \mathcal{N}_+}{N}} \quad b_p = \sqrt{\frac{N - \mathcal{N}_+}{N}} a_p$$

Remark: for all $p \in \Lambda_+^*$,

$$U^* b_p^* U = a_p^* \frac{a_0}{\sqrt{N}}$$

Hence b_p^* creates an excitation with momentum p and, at the same time, it annihilate a particle from the condensate.

Total number of particles is **conserved**. Moreover, on states with $\mathcal{N}_+ \ll N$, we expect $b_p \simeq a_p$, $b_p^* \simeq a_p^*$.

Generalized Bogoliubov transformations: let $w = 1 - f$ and

$$\eta_p = -\frac{1}{N^2} \hat{w}(p/N) \quad \Rightarrow \quad \eta_p \simeq \frac{C}{p^2}$$

We define

$$T = \exp \sum_{p \in \Lambda_+^*} \eta_p (b_p^* b_{-p}^* - b_p b_{-p}) : \mathcal{F}_+^{\leq N} \rightarrow \mathcal{F}_+^{\leq N}$$

Then

$$T^* b_p T = \cosh(\eta_p) b_p + \sinh(\eta_p) b_{-p}^* + d_p$$

where

$$\|d_p \xi\| \leq C N^{-1} \|(\mathcal{N}_+ + 1)^{3/2} \xi\|$$

Observe:

$$\begin{aligned} T^* \mathcal{N}_+ T &\simeq \mathcal{N}_+ + \|\eta\|_2^2 \simeq \mathcal{N}_+ + C \\ T^* \mathcal{K} T &\simeq \mathcal{K} + \|\eta\|_{H^1}^2 \simeq \mathcal{K} + C N \end{aligned}$$

T generates **finitely many** excitations but **macroscopic** energy.

Renormalized excitation Hamiltonian: define

$$\mathcal{G}_N = T^* \mathcal{L}_N T = T^* U H_N U^* T : \mathcal{F}_+^{\leq N} \rightarrow \mathcal{F}_+^{\leq N}$$

Using **cancellations** due to equation for η , we find

$$\mathcal{G}_N = 4\pi a_0 N + \mathcal{H}_N + \mathcal{E}_N$$

where $\mathcal{H}_N = \mathcal{K} + \mathcal{V}_N$ and, for every $\delta > 0$, there exists $C > 0$ with

$$\pm \mathcal{E}_N \leq \delta \mathcal{H}_N + C\kappa(\mathcal{N}_+ + 1)$$

Lower bound: since $\mathcal{N} \leq C\mathcal{K}$, we find

$$\mathcal{G}_N - 4\pi a_0 N \geq \frac{1}{2} \mathcal{H}_N - C$$

if $\kappa > 0$ is **small** enough.

Bose-Einstein condensation: if

$$\langle \psi_N, H_N \psi_N \rangle \leq 4\pi a_0 N + K,$$

the **excitation vector** $\xi_N = T^* U \psi_N$ is such that

$$K \geq \langle \psi_N, H_N \psi_N \rangle - 4\pi a_0 N = \langle \xi_N, \mathcal{G}_N \xi_N \rangle - 4\pi a_0 N \geq \frac{1}{2} \langle \xi_N, \mathcal{H}_N \xi_N \rangle - C$$

Hence, low energy states exhibit **BEC**, with optimal rate:

$$\langle \xi_N, \mathcal{N}_+ \xi_N \rangle \leq C \langle \xi_N, \mathcal{K} \xi_N \rangle \leq C \langle \xi_N, \mathcal{H}_N \xi_N \rangle \leq C(K + 1)$$

Stronger bound: if $\psi_N \in L^2(\Lambda)^{\otimes_s N}$ with

$$\psi_N = \chi(H_N \leq E_N + \zeta) \psi_N$$

Then $\psi_N = U_N^* T \xi_N$ with

$$\langle \xi_N, [(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1) + (\mathcal{N}_+ + 1)^3] \xi_N \rangle \leq C(\zeta + 1)^3$$

Proposition: the renormalized excitation Hamiltonian can be decomposed as

$$\mathcal{G}_N = C_N + \mathcal{Q}_N + \mathcal{C}_N + \mathcal{V}_N + \mathcal{E}_N$$

where C_N is a **constant**, \mathcal{Q}_N is **quadratic**,

$$\mathcal{C}_N = \frac{\kappa}{\sqrt{N}} \sum_{\substack{p, q \in \Lambda_+^* \\ q \neq -p}} \hat{V}(p/N) \left[b_{p+q}^* b_{-p}^* (\gamma_q b_q + \sigma_q b_{-q}^*) + \text{h.c.} \right]$$

and, where,

$$\pm \mathcal{E}_N \leq \frac{C}{\sqrt{N}} \left[(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1) + (\mathcal{N}_+ + 1)^3 \right]$$

Problem: \mathcal{G}_N still contains non-negligible **cubic** and **quartic** terms! This is the main difference compared with case $\beta < 1$!

Not surprising: from [Erdős-S.-Yau, 08], [Napiorkowski-Reuvers-Solovej, '15] it is clear that Bogoliubov states can only approximate ground state energy up to an **error** $\mathcal{O}(1)$.

Cubic phase: we define

$$A = \frac{1}{\sqrt{N}} \sum_{r \in P_H, v \in P_L} \eta_r \left[\sigma_v b_{r+v}^* b_{-r}^* b_{-v}^* + \gamma_v b_{r+v}^* b_{-r}^* b_v - \text{h.c.} \right]$$

with $P_L = \{p \in \Lambda_+^* : |p| \leq \sqrt{N}\}$, $P_H = \{p \in \Lambda_+^* : |p| \geq \sqrt{N}\}$.

Set $S = e^A$ and introduce **new excitation Hamiltonian**

$$\mathcal{J}_N = S^* T^* U_N H_N U_N^* T S : \mathcal{F}_+^{\leq N} \rightarrow \mathcal{F}_+^{\leq N}$$

Remark: a similar cubic conjugation was used in [Yau-Yin, 09].

Proposition: we can decompose

$$\mathcal{J}_N = \tilde{C}_N + \tilde{Q}_N + \mathcal{V}_N + \tilde{\mathcal{E}}_N$$

where \tilde{C}_N is a **constant**, \tilde{Q}_N is **quadratic** in creation and annihilation operators, and where

$$\pm \tilde{\mathcal{E}}_N \leq \frac{C}{N^{1/4}} \left[(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1) + (\mathcal{N}_+ + 1)^3 \right]$$

Diagonalization: quadratic term given by

$$\tilde{Q}_N = \sum_{p \in \Lambda_+^*} F_p b_p^* b_p + \frac{G_p}{2} [b_p b_{-p} + b_p^* b_{-p}^*]$$

with

$$F_p = p^2(\sigma_p^2 + \gamma_p^2) + \kappa(\hat{V}(\cdot/N) * \hat{f}_N)_p (\gamma_p + \sigma_p)^2;$$

$$G_p = 2p^2 \sigma_p \gamma_p + \kappa(\hat{V}(\cdot/N) * \hat{f}_N)_p (\gamma_p + \sigma_p)^2$$

We define new **Bogoliubov transformation**

$$\tanh(2\tau_p) = -\frac{G_p}{F_p} \quad \Rightarrow \quad R = \exp \left[\frac{1}{2} \sum_{p \in \Lambda_+^*} \tau_p (b_p^* b_{-p}^* - b_p b_{-p}) \right]$$

Then

$$R^* \tilde{Q}_N R = \frac{1}{2} \sum_{p \in \Lambda_+^*} \left[-F_p + \sqrt{F_p^2 - G_p^2} \right] + \sum_{p \in \Lambda_+^*} \sqrt{F_p^2 - G_p^2} a_p^* a_p + \delta_N$$

with

$$\pm \delta_N \leq CN^{-1}(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1)$$

Final excitation Hamiltonian: we define

$$\mathcal{M}_N = R^* \mathcal{J}_N R = R^* S^* T^* U_N H_N U_N^* T S R : \mathcal{F}_+^{\leq N} \rightarrow \mathcal{F}_+^{\leq N}$$

Then

$$\begin{aligned} \mathcal{M}_N = & 4\pi \mathfrak{a}_N (N - 1) \\ & + \frac{1}{2} \sum_{p \in \Lambda_+^*} \left[-p^2 - 8\pi \mathfrak{a}_0 + \sqrt{|p|^4 + 16\pi \mathfrak{a}_0 p^2} + \frac{(8\pi \mathfrak{a}_0)^2}{2p^2} \right] \\ & + \sum_{p \in \Lambda_+^*} \sqrt{|p|^4 + 16\pi \mathfrak{a}_0 p^2} a_p^* a_p + \mathcal{V}_N + \mathcal{E}'_N \end{aligned}$$

where

$$\pm \mathcal{E}'_N \leq C N^{-1/4} \left[(\mathcal{H}_N + 1)(\mathcal{N}_+ + 1) + (\mathcal{N}_+ + 1)^3 \right]$$

Main theorem follows from **min-max principle**, because on low-energy states of diagonal quadratic Hamiltonian, we find

$$\mathcal{V}_N \leq C N^{-1} (\zeta + 1)^{7/2}$$