Dynamical and Spectral Properties of Bose-Einstein Condensates

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Based on joint works with
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I. The Gross-Pitaevskii Limit

Hamiltonian: consider N particles described by

$$H_N^{\text{trap}} = \sum_{j=1}^{N} \left[-\Delta_{x_j} + V_{\text{ext}}(x_j) \right] + \sum_{i<j}^{N} N^2 V(N(x_i - x_j))$$

on $L_s^2(\mathbb{R}^{3N})$. Here $V \geq 0$, regular, radial, compactly supported.

Scattering length: defined by zero-energy scattering equation

$$\left[-\Delta + \frac{1}{2} V(x) \right] f(x) = 0, \qquad f(x) \to 1$$

For $|x|$ large,

$$f(x) = 1 - \frac{a_0}{|x|} \quad \Rightarrow \quad a_0 = \text{scattering length of } V$$

By scaling

$$\left[-\Delta + \frac{N^2}{2} V(Nx) \right] f(Nx) = 0 \quad \Rightarrow \quad \frac{a_0}{N} = \text{scatt. length of } N^2 V(N.)$$

Ground state energy: [**Lieb-Seiringer-Yngvason, '00**] proved

$$\lim_{N\to\infty} \frac{E_N}{N} = \min_{\varphi\in L^2(\mathbb{R}^3):\|\varphi\|=1} \int \left[|\nabla\varphi|^2 + V_{\text{ext}}|\varphi|^2 + 4\pi a_0 |\varphi|^4 \right] dx$$

Bose-Einstein condensation: let

$$\gamma_N^{(1)} = \text{Tr}_{2,\dots,N} |\psi_N\rangle\langle\psi_N|$$

be one-particle marginal associated with ground state ψ_N.

[**Lieb-Seiringer, '02**] proved that

$$\gamma_N^{(1)} \to |\varphi_0\rangle\langle\varphi_0|, \qquad \text{where } \varphi_0 \text{ minimizes GP-energy.}$$

Warning: this does not mean that $\psi_N \simeq \varphi_0^{\otimes N}$. In fact

$$\frac{1}{N}\left\langle \varphi_0^{\otimes N}, H_N^{\text{trap}}\, \varphi_0^{\otimes N} \right\rangle \simeq \int \left[|\nabla\varphi_0|^2 + V_{\text{ext}}|\varphi_0|^2 + \frac{\widehat{V}(0)}{2}|\varphi_0|^4 \right] dx$$

Correlations are crucial!

II. Time-evolution of BEC

$$\text{Let} \qquad H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^2 V(N(x_i - x_j)).$$

Theorem [Brennecke - S., '17]: Let $\psi_N \in L^2_s(\mathbb{R}^{3N})$ such that

$$a_N := \text{Tr} \left| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right| \to 0$$

$$b_N := \left| \frac{1}{N} \langle \psi_N, H_N \psi_N \rangle - \int \left[|\nabla \varphi|^2 + 4\pi a_0 |\varphi|^4 \right] \right| \to 0$$

as $N \to \infty$. Let $\psi_{N,t} = e^{-iH_N t} \psi_N$. Then, for all $t \in \mathbb{R}$,

$$1 - \langle \varphi_t, \gamma_{N,t}^{(1)} \varphi_t \rangle \leq C(a_N + b_N + N^{-1}) \exp(c \exp(c|t|))$$

where φ_t solves **time-dependent Gross-Pitaevskii** equation

$$i\partial_t \varphi_t = \left[-\Delta + V_{\text{ext}}(x) \right] \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t$$

with initial data $\varphi_{t=0} = \varphi$.

Remark: result immediately implies

$$\text{Tr}\left|\gamma_{N,t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|\right| \leq C(a_N + b_N + N^{-1})^{1/2}\exp(c\exp(c|t|))$$

Previous works:

[**Erdős-S.-Yau, '06-'08**]: BBGKY approach, no information on rate of convergence

[**Pickl, '10**]: alternative approach, uncontrolled rate of convergence

[**Benedikter-de Oliveira-S. '12**]: precise bounds on rate, approximately coherent initial data in Fock space.

Orthogonal excitations: for $\psi_N \in L^2_s(\mathbb{R}^{3N})$ and $\varphi \in L^2(\mathbb{R}^3)$, write

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

where $\alpha_j \in L^2_{\perp\varphi}(\mathbb{R}^3)^{\otimes_s j}$.

As in [**Lewin-Nam-Serfaty-Solovej, '12**], [**Lewin-Nam-S. '15**], we define unitary map

$$\begin{aligned} U_\varphi : L^2_s(\mathbb{R}^{3N}) \to \mathcal{F}^{\leq N}_{\perp\varphi} &= \bigoplus_{j=0}^{N} L^2_{\perp\varphi}(\mathbb{R}^3)^{\otimes_s j} \\ \psi_N \to U_\varphi \psi_N &= \{\alpha_0, \alpha_1, \dots, \alpha_N\} \end{aligned}$$

Remark: $\psi_N = U^*_\varphi \xi_N$ exhibits BEC if and only if $\xi_N \in \mathcal{F}^{\leq N}_{\perp\varphi}$ has small number of particles.

Evolution of BEC: define **excitation vector** $\widetilde{\xi}_{N,t} \in \mathcal{F}^{\leq N}_{\perp \varphi_t}$ through

$$e^{-iH_N t} U^*_{\varphi} \, \xi_N = U^*_{\varphi_t} \, \widetilde{\xi}_{N,t}$$

In other words,

$$\widetilde{\xi}_{N,t} = \widetilde{\mathcal{W}}_{N,t} \xi_N$$

with **fluctuation dynamics**

$$\widetilde{\mathcal{W}}_{N,t} = U_{\varphi_t} \, e^{-iH_N t} \, U^*_{\varphi} : \mathcal{F}^{\leq N}_{\perp \varphi} \to \mathcal{F}^{\leq N}_{\perp \varphi_t}$$

Need to show

$$\langle \widetilde{\xi}_{N,t}, \mathcal{N} \widetilde{\xi}_{N,t} \rangle = \langle \xi_N, \widetilde{\mathcal{W}}^*_{N,t} \mathcal{N} \, \widetilde{\mathcal{W}}_{N,t} \, \xi_N \rangle \leq C_t$$

Problem: we are neglecting **correlations**!

Need to modify fluctuation dynamics!

Idea from [Benedikter-de Oliveira-S. '12]: interested in evolution of approximately **coherent initial data**:

$$e^{-i\mathcal{H}_N t} W_0 \, \xi_N = W_t \, \widetilde{\xi}_{N,t}, \qquad \text{with } W_t = \text{Weyl operator}$$

Describe correlations through **Bogoliubov transformations**

$$\widetilde{T}_t = \exp\left[\frac{1}{2}\int dxdy \, \left(\eta_t(x;y) a_x^* a_y^* - \text{h.c.}\right)\right]$$

Define **modified excitation vector** $\widetilde{\xi}_{N,t}$ through

$$e^{-i\mathcal{H}_N t} W_0 \, \widetilde{T}_0 \, \xi_N = W_t \, \widetilde{T}_t \, \xi_{N,t}$$

With choice

$$\widetilde{\eta}_t(x;y) = -Nw(N(x-y))\varphi_t(x)\varphi_t(y)$$

we obtain $\langle \xi_{N,t}, \mathcal{N} \xi_{N,t} \rangle \leq C_t$.

Goal: apply similar idea for N-particles data. **Problem**: Bogoliubov transformations do not leave $\mathcal{F}_{\perp \varphi_t}^{\leq N}$ invariant.

Modified fields: on $\mathcal{F}^{\leq N}_{\perp \varphi_t}$, we define, for $f \in L^2_{\perp \varphi_t}(\mathbb{R}^3)$,

$$b^*(f) = a^*(f) \sqrt{\frac{N - \mathcal{N}}{N}}, \qquad b(f) = \sqrt{\frac{N - \mathcal{N}}{N}} \, a(f)$$

Remark that

$$U^*_{\varphi_t} b^*(f) U_{\varphi_t} = a^*(f) \frac{a(\varphi_t)}{\sqrt{N}}$$

Hence $b^*(f)$ **creates** an excitation and, at the same time, it **annihilates** a particle in condensate.

Generalized Bogoliubov transformations: define

$$T_t = \exp \left[\frac{1}{2} \int dx dy \, \left(\eta_t(x;y) b^*_x b^*_y - \text{h.c.} \right) \right]$$

Then $T_t : \mathcal{F}^{\leq N}_{\perp \varphi_t} \to \mathcal{F}^{\leq N}_{\perp \varphi_t}$.

Modified fluctuation dynamics: let

$$\mathcal{W}_{N,t} = T_t^* \, U_{\varphi_t} \, e^{-iH_N t} \, U_\varphi^* \, T_0 : \mathcal{F}_{\perp\varphi}^{\leq N} \to \mathcal{F}_{\perp\varphi_t}^{\leq N}$$

Generator: define $\mathcal{G}_{N,t}$ such that

$$i\partial_t \mathcal{W}_{N,t} = \mathcal{G}_{N,t} \mathcal{W}_{N,t}$$

We find

$$\mathcal{G}_{N,t} = C_{N,t} + \mathcal{H}_N + \mathcal{E}_{N,t}$$

with

$$\mathcal{H}_N = \int \nabla_x a_x^* \nabla_x a_x + \frac{1}{2} \int dx dy \, N^2 V(N(x-y)) a_x^* a_y^* a_y a_x$$

and, for any $\delta > 0$, a $C > 0$ s.t.

$$\begin{aligned} \pm \, \mathcal{E}_{N,t} &\leq \delta \mathcal{H}_N + C(\mathcal{N} + 1) \\ \pm \left[\mathcal{E}_{N,t}, i\mathcal{N} \right] &\leq \delta \mathcal{H}_N + C(\mathcal{N} + 1) \\ \pm \, d\mathcal{E}_{N,t}/dt &\leq \delta \mathcal{H}_N + C(\mathcal{N} + 1) \end{aligned}$$

Control of $\mathcal{N}$: by **Gronwall**, we conclude

$$\langle \xi_N, \mathcal{W}^*_{N,t} \mathcal{N} \, \mathcal{W}_{N,t} \, \xi_N \rangle \leq C_t \langle \xi_N, (\mathcal{N} + \mathcal{H}_N) \, \xi_N \rangle$$

With assumptions on initial data, theorem follows.

Main challenge: action of Bogoliubov transf. $\widetilde{T}_t$ is explicit, i.e.

$$\widetilde{T}_t \, a^*(f) \, \widetilde{T}_t = a^*(\cosh_{\eta_t} f) + a(\sinh_{\eta_t}(\bar{f}))$$

For generalized Bogoliubov transformations, **no explicit formula** is available.

Instead, we **expand**

$$T_t^* \, a^*(f) \, T_t = \sum_{n \geq 0} \frac{1}{n!} \mathrm{ad}^{(n)}(a^*(f))$$

III. Spectral properties of Bose gases

Consider N bosons in $\Lambda = [0;1]^{\times 3}$, periodic boundary conditions.

Hamiltonian: In **momentum space**, with $\Lambda^* = 2\pi\mathbb{Z}^3$, we have

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

for coupling constant $\kappa > 0$.

For $p \in \Lambda^*$, a_p^*, a_p are creation and annihilation operators, with

$$\left[a_p, a_q^*\right] = \delta_{p,q}, \qquad \left[a_p, a_q\right] = \left[a_p^*, a_q^*\right] = 0$$

From [**Lieb-Seiringer-Yngvason '00**], [**Lieb-Seiringer '02**],

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

and

$$\gamma_N^{(1)} \to |\varphi_0\rangle\varphi_0|$$

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

Mean-field regime: for

$$H_N^{\text{mf}} = \sum_{p\in\Lambda^*} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r\in\Lambda^*} \widehat{V}(r) a_{p+r}^* a_q^* a_p a_{q+r}$$

more information is available; [**Seiringer**], [**Grech-Seiringer**], [**Lewin-Nam-Serfaty-Solovej**], [**Derezinski-Napiorkowski**], [**Pizzo**].

Strong BEC bounds: $1 - \langle \varphi_0, \gamma_N^{(1)} \varphi_0 \rangle \leq C N^{-1}$

Precise ground state energy estimate: we find

$$E_N^{\text{mf}} = \frac{(N-1)\widehat{V}(0)}{2} - \frac{1}{2} \sum_{p\in\Lambda_+^*} \left[p^2 + \kappa \widehat{V}(p) - \sqrt{|p|^4 + 2\kappa p^2 \widetilde{V}(p)} \right] + o(1)$$

Low-lying excitation spectrum: consists of finite sums

$$\sum_{p\in\Lambda_+^*} n_p \sqrt{|p|^4 + 2\kappa p^2 \widehat{V}(p)} + o(1), \qquad \text{with } n_p \in \mathbb{N}$$

Natural question: can we establish **Bogoliubov theory** for **Gross-Pitaevskii regime** as well?

Theorem [Boccato - Brennecke - Cenatiempo - S., '17]: Suppose $\kappa > 0$ is small enough. Let $\psi_N \in L^2_s(\Lambda^N)$ such that

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

Then there exists $C > 0$ such that

$$1 - \langle \varphi_0, \gamma_N^{(1)} \varphi_0 \rangle \leq \frac{C(K+1)}{N}$$

Excitation Hamiltonian: we use unitary map

$$U : L^2_s(\Lambda^N) \to \mathcal{F}_+^{\leq N} = \bigoplus_{n=0}^{N} L^2_{\perp \varphi_0}(\Lambda)^{\otimes_s n}$$

to define

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

A long but straightforward computation shows that

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

where $\Lambda_+^* = \Lambda^*\backslash\{0\} = 2\pi\mathbb{Z}^3\backslash\{0\}$.

Remark: applying U reminds of **Bogoliubov approximation**.

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

Modified excitation Hamiltonian: let

$$\eta_p = -\frac{1}{N^2}\widehat{w}(p/N) \qquad \left(\text{so that } \eta_p \simeq \frac{Ca_0}{p^2}\right)$$

and construct **generalized Bogoliubov transformation**

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

We define then

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

Bounds on excitation Hamiltonian: as in dynamics, we find

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

where

$$\mathcal{H}_N = \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q \in \Lambda_+^*, r \in \Lambda^* : r \neq -p,-q} \widehat{V}(r/N) a_{p+r}^* a_q^* a_p a_{q+r}$$

and $\mathcal{E}_N$ is such that, for every $\delta > 0$, there exists $C > 0$ such that

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

Observation: kinetic energy has a **gap**, i.e.

$$\mathcal{K} = \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p \geq (2\pi)^2 \mathcal{N}$$

Hence

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

Next question: is strong BEC enough to establish Bogoliubov theory for **excitation spectrum** in Gross-Pitaevskii regime?

Answer: **no**, some of higher order terms in $\mathcal{G}_N$ are not negligible, for $N \to \infty$.

Not surprising: quasi-free states can only approximate ground state energy up to errors of order one [**Erdős-S.-Yau, '08**], [**Napiorkowski-Reuvers-Solovej, '15**]

Intermediate regimes: for $\beta \in [0;1]$, let

$$H_N^\beta = \sum_{p \in \Lambda^*} p^2 a_p^* a_p + \frac{1}{2N} \sum_{p,q,r \in \Lambda^*} \widehat{V}(r/N^\beta) a_{p+r}^* a_q^* a_p a_{q+r}$$

Notice: $\beta = 0$ is mean field, $\beta = 1$ is Gross-Pitaevskii regime.

Theorem [Boccato - Brennecke - Cenatiempo - S. '17]:
Let $0 < \beta < 1$. Let $\kappa > 0$ be small enough. Then

$$E_N^\beta = 4\pi a_N^\beta (N-1) - \frac{1}{2}\sum_{p\in\Lambda_+^*}\left[p^2 + \kappa\widehat{V}(0) - \sqrt{|p|^4 + 2\kappa p^2 \widehat{V}(0)} - \frac{\kappa^2 \widehat{V}^2(0)}{2p^2}\right] + o(1)$$

where

$$8\pi a_N^\beta = \kappa\widehat{V}(0) - \frac{1}{2N}\sum_{p\in\Lambda_+^*}\frac{\kappa^2\widehat{V}^2(p/N^\beta)}{p^2} + \sum_{k=2}^m \frac{(-1)^k\kappa^k}{(2N)^k}\sum_{p_i\in\Lambda_+^*}\frac{\widehat{V}(p_1/N^\beta)}{p_1^2}\left[\prod_{i=1}^{k-1}\frac{\widehat{V}((p_i - p_{i+1})/N^\beta)}{p_{i+1}^2}\right]\widehat{V}(p_k/N^\beta)$$

Moreover, spectrum of $H_N^\beta - E_N^\beta$ below K consists of

$$\sum_{p\in\Lambda_+^*} n_p\sqrt{|p|^4 + 2\kappa p^2\widehat{V}(0)} + o(1), \qquad \text{with } n_p \in \mathbb{N}$$

Remark: k-th term in **Born series** gives contribution $\mathcal{O}(N^{k\beta-(k-1)})$. Hence, for $\beta < 1$, series can be truncated at finite order.

Excitation Hamiltonian: we define

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

As before

$$\mathcal{G}_N^\beta = 4\pi a_N^\beta N + \mathcal{H}_N^\beta + \mathcal{E}_N^\beta$$

where

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

This implies that **low-energy** states $\psi_N = U^* T \xi_N$ are so that

$$\langle \xi_N, \mathcal{N} \xi_N \rangle \leq C$$

and, with some more work, that

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

Quadratic Hamiltonian: more **careful analysis** shows

$$\mathcal{G}_N^\beta = C_N + \sum_{p\in\Lambda_+^*} F_p \, b_p^* \, b_p + \frac{G_p}{2} \left[b_p^* b_{-p}^* + b_p b_{-p} \right] + \delta_N^\beta$$

$$=: C_N + \mathcal{Q} + \delta_N^\beta$$

where

$$F_p = p^2(\sinh^2 \eta_p + \cosh^2 \eta_p) + \kappa \widehat{V}(p/N^\beta)(\sinh \eta_p + \cosh \eta_p)^2$$

$$G_p = 2p^2 \sinh \eta_p \cosh \eta_p + \kappa \widehat{V}(p/N^\beta)(\sinh \eta_p + \cosh \eta_p)^2 + \frac{\kappa}{N} \sum_{q\in\Lambda_+^*} \widehat{V}((p-q)/N^\beta)\eta_q$$

and

$$\pm\delta_N^\beta \le C N^{-\alpha}(\mathcal{N}+1)(\mathcal{H}_N+1)$$

for some $\alpha > 0$.

Diagonalization: for $p \in \Lambda_+^*$, let τ_p s.t.

$$\tanh \tau_p = \frac{G_p}{F_p}$$

Define **generalized Bogoliubov transformation**

$$S = \exp\left[\frac{1}{2}\sum_{p\in\Lambda_+^*} \tau_p (b_p^* b_{-p}^* - b_p b_{-p})\right]$$

so that

$$S^* \mathcal{Q} S = \sum_{p\in\Lambda_+^*} \left[-\frac{F_p}{2} + \sqrt{F_p^2 - G_p^2}\right] + \sum_{p\in\Lambda_+^*} \sqrt{F_p^2 - G_p^2}\, a_p^* a_p + \delta_{\mathcal{Q}}$$

with

$$\pm\,\delta_{\mathcal{Q}} \leq C N^{-1} (\mathcal{N} + 1)(\mathcal{H}_N + 1)$$

Diagonal excitation Hamiltonian: we define

$$\mathcal{M}_N = S^* \mathcal{G}_N^{\beta} S = S^* T^* U H_N U^* T S : \mathcal{F}_+^{\leq N} \to \mathcal{F}_+^{\leq N}$$

Then

$$\begin{aligned}\mathcal{M}_N^{\beta} &= 4\pi a_N^{\beta}(N-1) \\ &\quad - \frac{1}{2} \sum_{p \in \Lambda_+^*} \left[p^2 + \kappa \widehat{V}(0) - \sqrt{|p|^4 + 2\kappa p^2 \widehat{V}(0)} - \frac{\kappa^2 \widehat{V}^2(0)}{2p^2} \right] \\ &\quad + \sum_{p \in \Lambda_+^*} \sqrt{|p|^4 + 2\kappa p^2 \widehat{V}(0)}\, a_p^* a_p + \widetilde{\delta}_N^{\beta}\end{aligned}$$

with

$$\pm \widetilde{\delta}_N^{\beta} \leq C N^{-\alpha} (\mathcal{N} + 1)(\mathcal{H}_N + 1)$$

Important ingredient: $F_p \simeq p^2$, $G_p \simeq 1/p^2$, and hence $\tau_p \simeq |p|^{-4}$. Therefore S "**preserves**" $\mathcal{N}$ and also $\mathcal{H}_N$!