The dynamics of weakly interacting trapped Bose gases at positive temperature

Andreas Deuchert

Institute of Mathematics, University of Zurich (UZH)

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The model

The **Hamiltonian** in mean-field (MF) scaling is given by

$$H_N = \sum_{i=1}^{N} (-\Delta_i + w(x_i)) + \frac{1}{N} \sum_{1 \leq i < j \leq N} v(x_i - x_j).$$

At temperature $T > 0$ the system is described by the **free energy** and the **Gibbs state**

$$F(T, N) = -T \ln \mathrm{Tr}[\exp(-H_N/T)] \quad \text{and} \quad \Gamma_{\mathrm{G}} = \frac{\exp(-H_N/T)}{\mathrm{Tr}[\exp(-H_N/T)]},$$

respectively. The traces are taken over **permutation symmetric functions**. We have

$$\lim_{T \to 0} F(T, N) = E_N \quad \text{and} \quad \lim_{T \to 0} \Gamma_{\mathrm{G}} = |\Psi_N\rangle\langle\Psi_N|,$$

where E_N denotes the **lowest eigenvalue** of H_N and $H_N \Psi_N = E_N \Psi_N$.

1-pdm and BEC

The **one-particle reduced density matrix (1-pdm)** of the Gibbs state Γ_{G} can be defined via its integral kernel

$$\gamma_{\mathrm{G}}(x,y) = N \int \Gamma_{\mathrm{G}}(x, q_1, ..., q_{N-1}; y, q_1, ..., q_{N-1}) \,\mathrm{d}(q_1, ..., q_{N-1}).$$

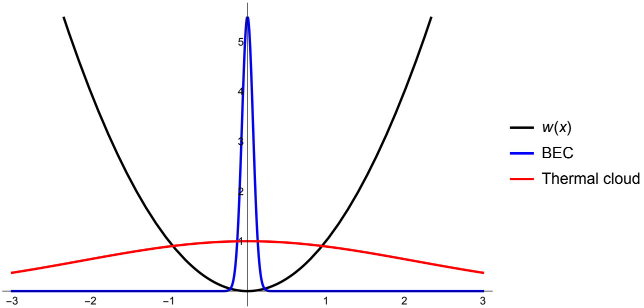
It is the quantum version of the **one-particle marginal** of an N-particle probability distribution.

We say that Γ_{G} displays **Bose–Einstein condensation (BEC)** iff

$$\liminf_{N\to\infty} \sup_{\|\phi\|_{L^2(\mathbb{R}^3)}} \frac{\langle \phi, \gamma_{\mathrm{G}} \phi \rangle}{N} > 0.$$

Scales for ideal Bose gas with $w(x) = |x|^s$ and $s > 0$

Critical temperature of ideal gas: $T_c(s) = C(s)N^{\alpha}$ with $\alpha = \frac{2s}{6+3s}$.



- Free energy $F_0(T, N) \sim TN \sim N^{1+\alpha}$
- Length scale density condensate: 1
- Length scale density thermal cloud: $N^{\frac{\alpha}{s}}$

The interacting problem at $T > 0$

$$E^{\mathrm{H}}(g) = \inf_{\|\phi\|=1} \left\{ \langle \phi, (-\Delta + w)\phi \rangle + \frac{g}{2} \int_{\mathbb{R}^6} |\phi(x)|^2 v(x-y) |\phi(y)|^2 \right\}$$

Natural scaling limit:

- $N \to \infty$
- $T \lesssim T_{\mathrm{c}}(s) \sim N^{\frac{2s}{6+3s}}$

Ideal gas quantities:

- $F_0(T, N)$
- $g = \lim_{N\to\infty} N_0(T, N)/N$

Theorem (Proved for harmonic trap)

We have

$$\lim_{N\to\infty} N^{-1} \left| F(T,N) - F_0(T,N) - NgE^{\mathrm{H}}(g) \right| = 0$$

as well as

$$\lim_{N\to\infty} N^{-1} \left\| \gamma_{\mathrm{G}} - \gamma^{\mathrm{id}} - Ng \left| \Phi_g^{\mathrm{H}} \right\rangle \left\langle \Phi_g^{\mathrm{H}} \right| \right\|_1 = 0.$$

Reference:

- A. D., R. Seiringer, J. Funct. Anal. 281, Issue 6, (2021)

Initial datum I: Reference state

We want to construct **perturbations** of the state

$$\Gamma(\phi, \gamma) = W(\phi) G(\gamma) W^*(\phi),$$

where $G(\gamma)$ is the unique **quasi-free state** on the bosonic Fock space $\mathscr{F}(L^2(\mathbb{R}^3))$ with 1-pdm γ that satisfies $[\mathcal{N}, G] = 0$. Moreover,

$$W(\phi) = \exp(a^*(\phi) - a(\phi))$$

is a **Weyl transformation** that implements the condensate. We call ϕ the **condensate wave function** and γ the 1-pdm of the **thermal cloud**. The expected number of particles in the state $\Gamma(\phi, \gamma)$ equals

$$\mathrm{Tr}_{\mathscr{F}}[\mathcal{N}\Gamma(\phi, \gamma)] = \int_{\mathbb{R}^3} |\phi(x)|^2 \, \mathrm{d}x + \mathrm{Tr}_{L^2(\mathbb{R}^3)}[\gamma] = N.$$

Initial datum II: Araki–Woods representation

We write $G(\gamma) = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|$ and define the **vector**

$$\Psi_G(\gamma) = \sum_{\alpha=1}^{\infty} \sqrt{\lambda_\alpha}\Psi_\alpha \otimes \overline{\Psi_\alpha} \in \mathscr{F}(L^2(\mathbb{R}^3)) \otimes \mathscr{F}(L^2(\mathbb{R}^3)).$$

This allows us to write

$$\mathrm{Tr}_{\mathscr{F}}[AG(\gamma)] = \langle \Psi_G(\gamma), (A \otimes \mathbb{1})\, \Psi_G(\gamma)\rangle$$

for $A \in \mathcal{B}(\mathscr{F})$. That is, we have represented $G(\gamma)$ as a **vector state** on the **doubled Fock space**. Moreover

$$\mathrm{Tr}_{\mathscr{F}}[A\Gamma(\phi,\gamma)] = \langle W(\phi) \otimes W(\overline{\phi})\Psi_G(\gamma), (A \otimes \mathbb{1})\, W(\phi) \otimes W(\overline{\phi})\Psi_G(\gamma)\rangle.$$

Reference:

- N. Benedikter, V. Jakšić, M. Porta, C. Saffirio, B. Schlein, Comm. Pure Appl. Math. **69**, no. 12, 2250 (2016).

Initial datum III: Exponential map

Let $\mathcal{U} : \mathscr{F}(L^2(\mathbb{R}^3)) \otimes \mathscr{F}(L^2(\mathbb{R}^3)) \to \mathscr{F}(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$ be the (unitary) **exponential map** defined by $\mathcal{U}\Omega \otimes \Omega = \widetilde{\Omega}$ and

$$\mathcal{U}\big(a(f) \otimes \mathbb{1}\big)\mathcal{U}^* = a(f \oplus 0) =: a_\ell(f),$$
$$\mathcal{U}\big(\mathbb{1} \otimes a(f)\big)\mathcal{U}^* = a(0 \oplus f) =: a_r(f).$$

We also define the **Weyl transformation**

$$\mathcal{W}(\phi) = \exp\big(a_\ell(\phi) + a_r(\overline{\phi}) - \mathrm{h.c.}\big)$$

acting on $\mathscr{F}(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$. Then

$$\mathrm{Tr}_{\mathscr{F}}[\mathcal{P}(a, a^*)\Gamma(\phi, \gamma)] = \langle \mathcal{U}\Psi_{\mathrm{G}}(\gamma), \mathcal{W}^*(\phi)\ \mathcal{P}(a_\ell, a_\ell^*)\ \mathcal{W}(\phi)\mathcal{U}\Psi_{\mathrm{G}}(\gamma)\rangle.$$

Initial datum IV: The perturbed state

With the **Bogoliubov transformation**

$$\mathcal{T}(\gamma) = \exp\left(\int_{\mathbb{R}^6} k_\gamma(x,y) a^*_{\ell,x} a^*_{r,y} \, \mathrm{d}(x,y) - \mathrm{h.c.} \right),$$

where $k_\gamma(x,y) = \mathrm{arcsinh}(\sqrt{\gamma})(x,y)$, we can write $\mathcal{U}\Psi_{\mathrm{G}}(\gamma) = \mathcal{T}(\gamma)\widetilde{\Omega}$, and hence

$$\mathrm{Tr}_{\mathscr{F}}[\mathcal{P}(a,a^*)\Gamma(\phi,\gamma)] = \langle \widetilde{\Omega}, \mathcal{T}^*(\gamma)\mathcal{W}^*(\phi)\mathcal{P}(a_\ell, a^*_\ell)\mathcal{W}(\phi)\mathcal{T}(\gamma)\widetilde{\Omega} \rangle.$$

The **perturbed state** $\Gamma_\xi(\phi,\gamma)$ is defined by

$$\mathrm{Tr}_{\mathscr{F}}[\mathcal{P}(a,a^*)\Gamma_\xi(\phi,\gamma)] = \langle \xi, \mathcal{T}^*(\gamma)\mathcal{W}^*(\phi)\mathcal{P}(a_\ell, a^*_\ell)\mathcal{W}(\phi)\mathcal{T}(\gamma)\xi \rangle$$

with $\xi \in \mathscr{F}(L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$.

Time evolution

We are interested in the solution to the **Heisenberg equation**

$$\mathrm{i}\partial_t \Gamma_{\xi,t} = [\mathcal{H}_N, \Gamma_{\xi,t}] \quad \text{with initial datum} \quad \Gamma_{\xi,0} = \Gamma_\xi(\phi,\gamma).$$

The **Hamiltonian** of the system is given by

$$\mathcal{H}_N = \int_{\mathbb{R}^3} \nabla a_x^* \nabla a_x \,\mathrm{d}x + \frac{1}{2N} \int_{\mathbb{R}^6} v(x-y) a_x^* a_y^* a_y a_x \,\mathrm{d}x \,\mathrm{d}y,$$

that is, we are interested in a **mean-field** system. The **time-evolved** state reads

$$\Gamma_{\xi,t} = \exp(-\mathrm{i}\mathcal{H}_{\mathcal{N}})\Gamma_\xi(\phi,\gamma)\exp(\mathrm{i}\mathcal{H}_{\mathcal{N}}).$$

In the **doubled Fock space picture** this reads

$$\mathrm{Tr}_{\mathscr{F}}[\mathcal{P}(a,a^*)\Gamma_{\xi,t}] = \langle \xi, \mathcal{T}^*(\gamma)\mathcal{W}^*(\phi)\exp(\mathrm{i}\mathcal{L}_N t)\mathcal{P}(a_\ell, a_\ell^*)\exp(-\mathrm{i}\mathcal{L}_N t)\mathcal{W}(\phi)\mathcal{T}(\gamma)\xi\rangle,$$

where $\mathcal{L}_N = \mathcal{H}_{N,\ell} - \mathcal{H}_{N,r}$.

Assumptions

Assumptions (Initial datum)

We assume that the pair (ϕ, γ) satisfies $n(\phi, \gamma) = N$ and that:

(A) *The* **condensate wave function** *ϕ can be written as the product of an N-dependent constant $c(N)$, which determines the expected number of particles in the condensate, times an N-independent function $\widetilde{\phi} \in L^2(\mathbb{R}^3)$.*

(B) *The* **1-pdm** *γ obeys*

$$\int_{\mathbb{R}^6} |\hat{\gamma}(p, q)| \, \mathrm{d}(p, q) \lesssim T_{\mathrm{c}}^{3/2}(s)$$

with $T_{\mathrm{c}}(s)$ above, and where $\hat{\gamma}(p, q)$ denotes the integral kernel of γ in Fourier space.

(C) *The* **operator norm** *of γ satisfies*

$$\|\gamma\| \lesssim T_{\mathrm{c}}(s).$$

Main result

Theorem

Let the **pair** (ϕ, γ) *satisfy the* **above assumptions** *with* $0 < s \leq 3/2$. *The* **fluctuation vector** ξ *is assumed to satisfy* $\langle \xi, (\mathcal{N}_\ell + \mathcal{N}_r)^{44} \xi \rangle \lesssim 1$.

Then the 1-pdm $\gamma_{\xi,t}$ *of the state* $\Gamma_{\xi,t}$ *satisfies*

$$\left\| \gamma_{\xi,t} - e^{\mathrm{i}\Delta t} \gamma e^{-\mathrm{i}\Delta t} - |\phi_t\rangle\langle\phi_t| \right\|_1 \lesssim_t \sqrt{N} T_{\mathrm{c}}^{3/4}(s),$$

where $\| \cdot \|_1$ *denotes the trace norm. The function* ϕ_t *is the solution to the* **time-dependent Hartree equation**

$$\mathrm{i}\partial_t \phi_t(x) = \left(-\Delta + N^{-1} v * |\phi_t(x)|^2\right) \phi_t(x) \quad \textit{with initial datum} \quad \phi_0(x) = \phi(x).$$

Reference:

- M. Caporaletti, A. D., B. Schlein, arXiv:2203.17204 [math-ph] (2022)

Remarks

- First result for dynamics of BEC with a **macroscopic number** of excited particles.
- Obtain an **optimal** N-dependence for the remainder for our set of initial data if we choose a slightly more general effective dynamics.
- The assumption for ξ with the 44th moment is the **worst case scenario** happening for $s = 3/2$.
- There is **no reason** to believe that the same result should not hold for all $s > 0$.
- Proof is based on the definition of **fluctuation dynamics** using the **Hartree–Fock–Bogoliubov (HFB) equations.**

Selected literature on MF dynamics

Convergence towards Hartree

- Hepp (1974); Ginibre, Velo (1979); Spohn (1980); Bardos, Golse, Mauser (2000); Erdös, Yau (2001); Elgart, Schlein (2007); Fröhlich, Knowles, Pizzo (2007); Fröhlich, Knowles, Schwarz (2009); Rodnianski, Schlein (2009); Knowles, Pickl (2010); Chen, Lee, Schlein (2011); Ammari, Falconi, Pawilowski (2016)

Fluctuations around Hartree

- Hepp (1974); Grillakis, Machedon, Margetis (2010, 2011); Ben Arous, Kirkpatrick, Schlein (2013); Buchholz, Saffirio, Schlein (2014); Lewin, Nam, Schlein (2015); Bossmann, Pavlović, Pickl, Soffer (2020)

Correlation fcts. for bosons and semiclassical MF limit for fermions

- Narnhofer, Sewell (1981); Benedikter, Porta, Schlein (2013); Petrat, Pickl (2014); Benedikter, Jakšić, Porta, Saffirio, Schlein (2016); Porta, Rademacher, Saffirio, Schlein (2016); Fröhlich, Knowles, Schlein, Sohinger (2019); Chong, Lafleche, Saffirio (2021)

Lecture notes and reviews

- Benedikter, Porta, Schlein (2016); Napiórkowski (2021)

Hartree–Fock–Bogoliubov (HFB) equations

For the triple $(\phi_t, \gamma_t, \alpha_t)$ consisting of a **condensate wave function** $\phi_t \in L^2(\mathbb{R}^3)$, a **positive trace class operator** γ_t (a 1-pdm), and a **pairing function** $\alpha_t \in L^2(\mathbb{R}^6)$, the **HFB equations** take the form

$$\begin{aligned} \mathrm{i}\partial_t \phi_t &= h(\gamma_t)\phi_t + k(\alpha_t^{\phi_t})\overline{\phi_t} \\ \mathrm{i}\partial_t \gamma_t &= [h(\gamma_t^{\phi_t}), \gamma_t] + k(\alpha_t^{\phi_t})\alpha_t^* - \alpha_t k(\alpha_t^{\phi_t})^* \\ \mathrm{i}\partial_t \alpha_t &= [h(\gamma_t^{\phi_t}), \alpha_t]_+ + [k(\alpha_t^{\phi_t}), \gamma_t]_+ + k(\alpha_t^{\phi_t}) \end{aligned}$$

with $[A,B]_+ = AB^T + BA^T$, $\gamma^\phi = \gamma + |\phi\rangle\langle\phi|$ and $\alpha^\phi = \alpha + |\phi\rangle\langle\overline{\phi}|$. Moreover, we use the notations

$$h(\gamma) = -\Delta + \frac{1}{N} v * \rho_\gamma + \frac{1}{N} v\sharp\gamma, \qquad k(\alpha) = \frac{1}{N} v\sharp\alpha,$$

where $v\sharp\sigma$ denotes the **operator with kernel** $v(x-y)\sigma(x,y)$, and the **density associated with the 1-pdm** γ is given by $\rho_\gamma(x) = \gamma(x,x)$.

Effective dynamics on doubled Fock space I

Let the **triple** $(\phi_t, \gamma_t, \alpha_t)$ be a **solution to the HFB equations** with initial datum $(\phi, \gamma, 0)$ and denote by

$$\Gamma_t^{(1)} = \begin{pmatrix} \gamma_t & \alpha_t \\ \overline{\alpha_t} & 1 - \overline{\gamma_t} \end{pmatrix}$$

the **generalized 1-pdm** of associated to $(\phi_t, \gamma_t, \alpha_t)$. Then there exists an **implementable symplectomorphism** $\mathcal{U}_t$ s.t.

$$\Gamma_t^{(1)} = \mathcal{U}_t^* \Gamma_0^{(1)} \mathcal{U}_t.$$

Reference:

- V. Bach, S. Breteaux, T. Chen, J. Fröhlich, I. M. Sigal, preprint arXiv:1602.05171 (2018).

Effective dynamics on doubled Fock space II

Let $\langle \cdot \rangle_t$ be the **unique quasi-free state** with

$$\langle a_x \rangle_t = \phi_t(x), \quad \langle a_y^* a_x \rangle_t - \langle a_y^* \rangle_t \langle a_x \rangle_t = \gamma_t(x,y), \qquad \text{and}$$
$$\langle a_x a_y \rangle_t - \langle a_x \rangle_t \langle a_y \rangle_t = \alpha_t(x,y).$$

If $\mathcal{R}_t$ is the **Bogoliubov transformation** implementing $\mathcal{U}_t$ and $\mathcal{T}_t = \mathcal{R}_t \mathcal{T}(\gamma)$, then

$$\langle \mathcal{P}(a, a^*) \rangle_t = \langle \widetilde{\Omega}, \mathcal{T}_t^* \mathcal{W}^*(\phi_t) \mathcal{P}(a_\ell, a_\ell^*) \mathcal{W}(\phi_t) \mathcal{T}_t \widetilde{\Omega} \rangle.$$

Fluctuation dynamics

The **fluctuation dynamics** is defined by

$$\mathcal{U}^{\mathrm{fluct}}(t,s) = \mathcal{T}_t^* \mathcal{W}^*(\phi_t) \exp(-\mathrm{i}\mathcal{L}_N(t-s)) \mathcal{W}(\phi_s) \mathcal{T}_s.$$

It allows us to write the 1-pdm $\gamma_{\xi,t}$ of the **solution** $\Gamma_{\xi,t}(\phi,\gamma)$ to the **Heisenberg equation** as

$$\begin{aligned} \gamma_{\xi,t}(x,y) &= \langle \xi_t, \mathcal{T}_t^* \mathcal{W}^*(\phi_t) a_{\ell,y}^* a_{\ell,x} \mathcal{W}(\phi_t) \mathcal{T}_t \xi_t \rangle \\ &= \phi_t(x) \overline{\phi_t(y)} + \gamma_t(x,y) \\ &\quad + \text{terms whose trace-norm can be bounded in terms of } \langle \xi_t, \mathcal{N} \xi_t \rangle \end{aligned}$$

with the **time-dependent fluctuation vector**

$$\xi_t = \mathcal{U}^{\mathrm{fluct}}(t,0)\xi.$$