Kinetic Description of a Homogeneous Bose Fluid with Condensate

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Dynamics of Bose-Einstein condensation?

A 3-dimensional Bose fluid exhibits Bose-Einstein condensation at low temperatures.

- Rigorous results in the Gross-Pitaevskii (mean-field) limit:
  - The limit is a factorized state, determined by the *condensate wave-function* [Lieb, Seiringer, Yngvason]
    $\Rightarrow$ 100% condensation, i.e., zero temperature
  - Time-evolution of a *spatially inhomogeneous* condensate wave-function determined by the Gross-Pitaevskii equation [Erdős, Schlein, Yau]
- No rigorous results for states with finite temperature (partial condensation).

Warmup: dNLS

Discrete nonlinear Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi_t(x) = \sum_{y\in\mathbb{Z}^d} \alpha(x-y)\psi_t(y) + \lambda|\psi_t(x)|^2\psi_t(x)$$

- $\psi_t : \mathbb{Z}^d \to \mathbb{C}, \quad t \in \mathbb{R}, \quad d \geq 1$
- $\lambda > 0$
- Harmonic couplings determined by $\alpha : \mathbb{Z}^d \to \mathbb{R}$.
- α sufficiently regular: finite range and sufficiently dispersive (for instance, nearest neighbor with $d \geq 4$)

Kinetic conjecture for homogeneous initial data

- Assume that the initial state is translation invariant
- Then there always exists $\tilde{w}_t(x)$, $x \in \mathbb{Z}^d$ such that

$$\mathbb{E}[\psi_t(x')^*\psi_t(x)] = \tilde{w}_t(x'-x)$$

- Kinetic conjecture: $W_\tau := \lim_{\lambda\to 0} \mathcal{F}\tilde{w}_{\tau\lambda^{-2}}$ solves a *homogeneous nonlinear Boltzmann-Peierls equation*

$$\partial_\tau W_\tau(k) = \mathcal{C}_{\mathrm{NL}}[W_\tau(\cdot)]\,,$$

$$\mathcal{C}_{\mathrm{NL}}[h](k_0) = 4\pi \int_{(\mathbb{T}^d)^3} \mathrm{d}k_1 \mathrm{d}k_2 \mathrm{d}k_3\, \delta(k_0+k_1-k_2-k_3)$$

$$\times\, \delta(\omega_0+\omega_1-\omega_2-\omega_3)\,[h_1 h_2 h_3 + h_0 h_2 h_3 - h_0 h_1 h_2 - h_0 h_1 h_3]\,,$$

$$h_j = h(k_j), \quad \omega_j = (\mathcal{F}\alpha)(k_j)$$

Moments to cumulants formula (cluster expansion)

Translation invariance important, leads to:

Cumulant expansion of initial time moments

For any index set I,

$$\mathbb{E}\Big[\prod_{i\in I}\widehat{\psi}_0(k_i,\sigma_i)\Big] = \sum_{S\in\pi(I)}\prod_{A\in S}\Big[\delta\Big(\sum_{i\in A}k_i\Big)C_{|A|}(k_A,\sigma_A)\Big],$$

where the sum runs over all partitions S of the index set I.

- Here *truncated correlation (cumulant) functions* are

$$C_n(k,\sigma) := \sum_{x\in(\mathbb{Z}^d)^n}\mathbb{1}(x_1=0)\mathrm{e}^{-\mathrm{i}2\pi\sum_{i=1}^n x_i\cdot k_i}\,\mathbb{E}\Big[\prod_{i=1}^n\psi_0(x_i,\sigma_i)\Big]^{\mathrm{trunc}}.$$

ℓ_1-clustering of the initial state

- For sufficiently small λ and for all $n \geq 4$ the fully truncated correlation functions (*cumulants*) should satisfy

$$\sup_{\Lambda,\sigma\in\{\pm 1\}^n} \sum_{x\in\Lambda^n} \mathbb{1}(x_1 = 0) \left| \mathbb{E}\left[\prod_{i=1}^n \psi_0(x_i,\sigma_i)\right]^{\text{trunc}} \right| \leq \lambda c_0^n n!$$

- For $n = 2$ should have

$$\sum_{\|x\|_\infty \leq L/2} \left| \mathbb{E}[\psi_0(0)^* \psi_0(x)] - \mathbb{E}[\psi_0(0)^* \psi_0(x)]_{L=\infty}^{\lambda=0} \right| \leq \lambda 2 c_0^2$$

- For a large class of dNLS equilibrium states proven by Abdesselam, Procacci, and Scoppola
- Estimates imply that $\|C_n\|_\infty < \infty$
  $\Rightarrow$ cumulant expansion encodes all singularities in k_i

Weakly interacting bosons

Consider a system of bosons "hopping" on a lattice $x \in \mathbb{Z}^d$, $d = 3$, and with weak "onsite" pair-interaction:

- Lattice convenient to avoid technicalities in the definitions
- The time-evolution lives in a Fock space, but conserves particle number.
- We consider N-particle Hamiltonians $H_N := H_N^{\text{free}} + \lambda V_N$,
  - $H_N^{\text{free}} = \sum_{j=1}^N \frac{1}{2}\Delta_j$, where Δ_j is a discrete Laplacian acting on the j:th particle
  - V_N is a multiplication operator by the pair-interaction potential $(x_1, \ldots, x_N) \mapsto \frac{1}{2}\sum_{i \neq j} \mathbb{1}(x_i - x_j = 0)$

Assume that the *initial state* is

1. *translation invariant*
2. ℓ_1*-clustering*: it has truncated correlation functions which decay summably

. . . follow a "nonlinear wave equation"

- Let $a(x)$ denote the *annihilation operator* at $x \in \mathbb{Z}^d$, and $a(x,t)$ denote the corresponding time-evolved operator.
- Then

$$\partial_t a(x,t) = -\mathrm{i}\sum_y \Delta(x-y)a(y,t) - \mathrm{i}\lambda a(x,t)^* a(x,t) a(x,t)$$

- For $a \to \psi$ equal to dNLS with $\alpha = \Delta$
- One important observable is *reduced 1-particle density matrix*,

$$\rho_1(x,y;t) = \langle a(y,t)^* a(x,t)\rangle$$

- By translation invariance, there is a function w such that

$$\rho_1(x,y;t) = w(x-y,t)$$

Kinetic conjecture

- Thus ($\hat{a}(k) := \sum_x \mathrm{e}^{-\mathrm{i}2\pi x\cdot k} a(x),\ k \in [0,1]^d$)

$$\langle \hat{a}(k,t)^* \hat{a}(k',t)\rangle = \delta(k-k')\hat{w}(k,t)$$
$$\langle \hat{a}(k',t) \hat{a}(k,t)^*\rangle = \delta(k-k')(1+\hat{w}(k,t))$$

- By perturbation expansion, one then expects that there exists a *kinetic scaling limit*

$$f(k,\tau) = \lim_{\lambda\to 0^+} \hat{w}(k,\tau\lambda^{-2})$$

  at least for not too large *kinetic times* $\tau > 0$.

- Moreover, the limit function should satisfy a nonlinear Boltzmann equation, $\partial_t f(k,t) = \mathcal{C}[f(\cdot,t)](k)$

Continuum, kinetic scaling limit, no condensate

In the corresponding *continuum setup* we get...

Nonlinear bosonic Boltzmann-Nordheim equation

$$\partial_t f(v_0, t) = \mathcal{C}_4[f(\cdot, t)](v_0), \quad v_0 \in \mathbb{R}^3,\ t > 0$$

$$\mathcal{C}_4[h](v_0) = 4\pi \int_{(\mathbb{R}^3)^3} \mathrm{d}v_1 \mathrm{d}v_2 \mathrm{d}v_3\, \delta(v_0 + v_1 - v_2 - v_3) \times \delta(\omega_0 + \omega_1 - \omega_2 - \omega_3) \left[\tilde{h}_0 \tilde{h}_1 h_2 h_3 - h_0 h_1 \tilde{h}_2 \tilde{h}_3\right],$$

$$h_j = h(v_j), \quad \tilde{h}_j = 1 + h_j, \quad \omega_j = E_j^{\mathrm{kin}} = \frac{1}{2} v_j^2$$

- *Identical* to the previous dNLS collision kernel, except here
  1. Different dispersion relation: $\omega(k) = \frac{1}{2} k^2$, with $k \in \mathbb{R}^3$
  2. Extra second order term: $h_2 h_3 - h_0 h_1$.

Homogeneous and isotropic distribution

Assume that f is also *isotropic in velocity*.

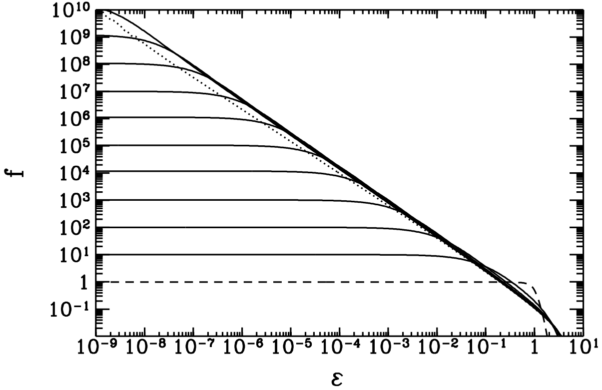
Define $f = f(x,t)$, $x = \omega(v) = \frac{1}{2}v^2$. Then,

$$\partial_t f(x,t) = \mathcal{C}_4[f(\cdot,t)](x)\,,$$

$$\mathcal{C}_4[h](x_0) = \frac{1}{\sqrt{x_0}} \int_{\mathbb{R}_+^2} \mathrm{d}x_2 \mathrm{d}x_3 \, \mathbb{1}(x_1 \geq 0) \min_{j=0,1,2,3} \sqrt{x_j}$$
$$\times \left[\tilde{h}_0 \tilde{h}_1 h_2 h_3 - h_0 h_1 \tilde{h}_2 \tilde{h}_3 \right]_{x_1 = x_2 + x_3 - x_0}$$

Asymptotics of solutions? Condensation?

Numerical results by Semikoz and Tkachev



Shows blow-up $f(0,t) \propto (t - t_0)^{-2.6}$ in finite time.
(dashed line depicts initial distribution)

Steady states

By differentiation of the integrand,

$$\partial_t s[f(\cdot,t)] = \sigma[f(\cdot,t)]\,,$$

$$s[h] = \int_0^\infty \mathrm{d}y \sqrt{y}\left[\tilde{h}(y)\ln\tilde{h}(y) - h(y)\ln h(y)\right], \quad (\textit{entropy})$$

$$\sigma[h] = \int_{\mathbb{R}_+^3} \mathrm{d}x_0\mathrm{d}x_2\mathrm{d}x_3\, \mathbb{1}(x_1 \geq 0) \min_{j=0,1,2,3}(\sqrt{x_j})\,(A-B)\ln\frac{A}{B},$$

$$A = \tilde{h}_0\tilde{h}_1 h_2 h_3, \quad B = h_0 h_1 \tilde{h}_2\tilde{h}_3, \qquad (\textit{entropy production})$$

Since $\sigma[f] \geq 0$, the steady states need to satisfy $\sigma[f] = 0$.
$\Rightarrow$ There are $\beta > 0$ and $\mu \leq 0$ such that $f = f_{\beta,\mu}$,

$$f_{\beta,\mu}(x) = \frac{1}{\mathrm{e}^{\beta(x-\mu)} - 1}$$

Conservation laws

For regular f, one similarly finds that particle number and energy are conserved: $\rho[f(t)], e[f(t)]$ are constant with

$$\rho[f] = \int_0^\infty \mathrm{d}y \sqrt{y}\, f(y)\,, \quad e[f] = \int_0^\infty \mathrm{d}y \sqrt{y}\, f(y) y$$

Definition

Given $f_0 = f(\cdot, 0)$, let $\bar{e} = e[f_0]$, and $\bar{\rho} = \rho[f_0]$.

1. *Either* $\exists!\ \beta, \mu$ such that $\bar{e} = e[f_{\beta,\mu}]$, and $\bar{\rho} = \rho[f_{\beta,\mu}]$,
2. *or* $\exists!\ \beta$ such that $\bar{e} = e[f_{\beta,0}]$, and $\bar{n} := \bar{\rho} - \rho_c > 0$, where $\rho_c = \rho[f_{\beta,0}]$.

   $\Rightarrow$ (?) steady state is $f(x)\sqrt{x}\mathrm{d}x = f_{\beta,0}(x)\sqrt{x}\mathrm{d}x + \bar{n}\,\delta(x)\mathrm{d}x$?

The importance of being earnestly defined

If $f(x,0)$ has a singularity, what is the proper mathematical definition of the evolution equation

$$\partial_t f(x,t) = \mathcal{C}_4[f(\cdot,t)](x)?$$

1. **Pointwise?** If $f_0(x) \simeq x^{-7/6}$ for $x \simeq 0$, then there is a unique (finite time) solution for which $f(x,t) \simeq b(t)x^{-7/6}$. [Escobedo, Mischler, Velázquez]

   However, this solution does not preserve total mass.

2. **Measure valued?** There is a family of positive measures $(\mu_t(\mathrm{d}x))_t$ which solve the equation weakly, and for which energy and mass are conserved. [Lu]

   Nonconstructive (via subsequences of solutions to a regularized problem); uniqueness?

Definition via physical ansatz

Semikoz and Tkachev (1997) used the following ansatz for numerical simulations:

$$f(x,t)\,\sqrt{x}\mathrm{d}x = f^{\mathrm{reg}}(x,t)\,\sqrt{x}\mathrm{d}x + n(t)\,\delta(x)\mathrm{d}x$$

yielding

$$\partial_t f^{\mathrm{reg}}(x,t) = \mathcal{C}_4[f_t^{\mathrm{reg}}](x) + n(t)\mathcal{C}_3[f_t^{\mathrm{reg}}](x),$$
$$\frac{\mathrm{d}}{\mathrm{d}t}n(t) = -n(t)\rho[\mathcal{C}_3[f_t^{\mathrm{reg}}]],$$

$$\mathcal{C}_3[h](x) = \frac{2}{\sqrt{x}}\int_0^x \mathrm{d}y\ \left[\tilde{h}(x)h(x-y)h(y) - h(x)\tilde{h}(x-y)\tilde{h}(y)\right]$$
$$-\frac{4}{\sqrt{x}}\int_x^\infty \mathrm{d}y\ [x \leftrightarrow y]$$

Effect of singularities in f_t

The following observations were made later by Spohn (2010):

- If $f(x,t) \simeq a(t)x^{-1}$ for $x \simeq 0$, then the condensate equation should read

$$\frac{\mathrm{d}}{\mathrm{d}t} n(t) = -n(t)\left(2\rho[\sqrt{x} f_t^{\mathrm{reg}}] - c_0 a(t)^2\right).$$

$\Rightarrow$ The previous measure-valued thermal states are stationary.

- If $f(x,t) \simeq b(t)x^{-7/6}$ for $x \simeq 0$, then

$$\rho[\mathcal{C}_4[f_t^{\mathrm{reg}}]] = -c_1 b(t)^3 .$$

$\Rightarrow$ Loss of mass, in spite of formal conservation law.

Final problem

How can condensate be generated? $(n(t) = 0 \;\Rightarrow\; \dot{n}(t) = 0)$

Possible scenario:

1. Start with supercritical but regular initial data $f(x, 0)$.
2. The solution to

$$\partial_t f(x, t) = \mathcal{C}_4[f(\cdot, t)](x)$$

   develops a singularity x^{-p}, $p > 1$, at $x = 0$ in finite time
3. After blowup: solution has x^{-1} singularity and a "seed" for condensate
4. Then $f(t), n(t)$ follow the coupled equations with $n(t) > 0$

Details of seeding poorly understood.
Not clear that condensation can be described by B-N eqn.

Evolution equations for f^{reg}

Possible solution:
Replace the equation for $\dot{n}$ by the mass conservation law,

$$n(t) = n(0) + \rho[f_0^{\mathrm{reg}}] - \rho[f_t^{\mathrm{reg}}] = \bar{n} - \rho[f_t^{\mathrm{reg}} - f_{\beta,0}]\,.$$

Evolution equation for the noncondensate energy density

$$\partial_t f^{\mathrm{reg}}(x,t) = \mathcal{C}_4[f_t^{\mathrm{reg}}](x) + (\bar{n} - \rho[f_t^{\mathrm{reg}} - f_{\beta,0}])\mathcal{C}_3[f_t^{\mathrm{reg}}](x)$$

- Closed nonlinear evolution equation for f^{reg}
- As a first step, we show that *small perturbations* from equilibrium have *unique solutions* converging to an equilibrium distribution as $t \to \infty$

Linearization

- Write $f^{\text{reg}} = f_{\beta,0} + R(x)\psi(t,x)$, $R(x) \propto x^{-1}$, and linearize:

$$\partial_t \psi_t = -L\psi_t + Q[\psi_t],$$
$$L = L_4 + \bar{n} L_3$$

- $f_{\beta,0}(x)$ has $1/x$ singularity for $x \to 0 \quad \Rightarrow$
  nonintegrable singularity $1/|x-y|$ for the integral kernel of L:

$$L_i\psi(x) = \int_0^\infty \mathrm{d}y\, K_i(x,y)(\psi(x) - \psi(y))\,, \quad i = 3, 4,$$
$$K_3 = x^{-\frac{1}{2}}|x-y|^{-1} \ \times \ (\text{exp-decay for } y > x),$$

and K_4 less singular ($\sim |x-y|^{-1/2}$).

Smoothing

Problem: nonlinear term *not bounded* in L^2 nor in Sobolev spaces.

- need *smoothing* by semigroup e^{-tL}
- L is close to a operator with *logarithmic* symbol $\sim \log(1+|\xi|)$, $\xi =$ Fourier-variable
- e^{-tL} smooths slowly, as $\sim |\xi|^{-t}$
- This is just what we need to "restore" the nonlinear term

Technical headache: singularity at origin (and at infinity)

Norms

To control all singularities, we work in *Banach spaces* X (for ψ) and X' (for $\partial_t\psi$), with *Hölder type* norms, $\frac{1}{2} < \alpha < 1$:

$$\|\psi\| = \sup_x |\psi(x)| + \|\psi\|', \quad \|\psi\|' \simeq \sup_{x,y} \frac{|\psi(x)-\psi(y)|}{|x-y|^\alpha} \frac{1}{\sqrt{x+y}},$$

$$\|\psi\|_{\ln} = \sup_x |\psi(x) \ln x^{-1}| + \|\psi\|'_{\ln},$$

$$\|\psi\|'_{\ln} \simeq \sup_{x,y} \frac{|\psi(x)-\psi(y)|}{|x-y|^\alpha \ln |x-y|^{-1}}$$

- Nonlinearity Q maps $X \to X'$ but
  $\int_0^t ds\, e^{-(t-s)L} Q[\psi_s]$ is a bounded map $X \to X$
- e^{-tL} has a "spectral" gap in X:
  $L : X \to X'$, $\|e^{-tL}\psi_0\| \le Ce^{-\delta t}\|\psi_0\|$ for some $\delta > 0$

Main novelty: analysis of the linear semigroup

- Why can do sup-norms?

  $\|\psi\| \leq \|\psi\|_{L^2} + \|\psi\|'$, $\quad \|\psi\|_{\ln} \leq \|\psi\|_{L^2} + \|\psi\|'_{\ln}$

- *The singularity at $x = 0$ enhances smoothing:*

  With $\psi_t = \mathrm{e}^{-tL}\psi_0$, $\Delta = |x - y|$, $\Phi_1(x, y) = (x + y)^{-1/2}$, $\alpha(x, y, t) = \alpha + \frac{1-\alpha}{2}\left(1 + [t\Phi_1(x, y)]^{-1}\right)^{-1}$, it holds

$$
\begin{aligned}
&|\psi_t(x) - \psi_t(y)| \\
&\qquad \leq \ln \Delta^{-1}\, \Delta^{\alpha(x,y,t)}(1 + t^2\Phi_1(x, y)^2)^{-1}\|\psi_0\|_{\ln}
\end{aligned}
$$

- *Gap in X* proven via similar *upper bound + gap in L^2*.

How are the upper bounds derived?

- Move $x = 0$ to $u = -\infty$: change variables to $u = \ln(e^x - 1)$
- Then $x^{-1/2} \to e^{-u/2}$
- Let $\Gamma_{uv}(t)$ denote the appropriate weight, and control

$$F_{uv}(t) := \frac{\psi_t(u) - \psi_t(v)}{\Gamma_{uv}(t)}, \qquad |u - v| \leq \varepsilon$$

which satisfies (with an explicit time-independent K_{uw})

$$\partial_t F_{uv} = F_{uv}\, \partial_t \ln \Gamma_{uv}^{-1} \\ -\Gamma_{uv}^{-1} \int dw\, [K_{uw}(\psi_t(u) - \psi_t(w)) - K_{vw}(\psi_t(v) - \psi_t(w))]$$

- Main observation: can generate a "potential term" by

$$\Gamma_{uv}^{-1}\left[A(\psi_t(u)-\psi_t(w))-B(\psi_t(v)-\psi_t(w))\right]$$
$$=F_{uv}\frac{2AB}{A+B}+\frac{A-B}{\Gamma_{uv}}\frac{A}{A+B}(\psi_t(u)-\psi_t(w))-(u\leftrightarrow v)$$

- The potential is singular on the diagonal $u \simeq v$

- Split the remaining integral over w into three parts
  1. Region dominated directly by the singular potential
  2. An integral containing $\int \mathrm{d}w\, \psi_t(w)\cdots$, use Schwarz ineq.
  3. For the rest, "telescope": $\psi_t(u)-\psi_t(w)=\sum_n F_{w_n,w_{n+1}}$

- For $|u-v| \le \varepsilon_0 \ll 1$ the singular potential dominates
  $\Rightarrow$ Banach fixed point theorem shows that $F_{uv}(t)$ is bounded
  $\Rightarrow$ proves that $\psi_t \in X$

Main mathematical result

Theorem

Let $\bar{n} > 0$ and suppose the initial data $f^{\mathrm{reg}}(x, 0)$ is such that $\|\psi_0\|$ is sufficiently small. Then there is a (unique) solution $f^{\mathrm{reg}}(x, t)$ which conserves total energy and mass and which converges exponentially fast to equilibrium: $f^{\mathrm{reg}} \to f_{\beta,0}, n(t) \to \bar{n}$ as $t \to \infty$.

Moreover, the equations derived by Spohn are satisfied and the corresponding family of measures provides a weak solution to the original Boltzmann equation, as considered by Lu.

Microscopic justification of the evolution equation?

$\partial_t f^{\text{reg}} = \mathcal{C}_4[f^{\text{reg}}] + n(t)\mathcal{C}_3[f^{\text{reg}}]$

- Assume that there is a density n_0 of particles in a state which has a "constant wavefunction"

  $\Rightarrow$ Then would expect an additional term in ρ_1:

$$\langle a(y,0)^* a(x,0)\rangle = n_0 + w(x-y,0)$$

- This leads to an initial state with

$$\langle a(k,0)^* a(k',0)\rangle = \delta(k'-k)\,[n_0\delta(k) + \hat{w}(k,0)]$$

- Can we still do the perturbation argument?

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