On the dynamics of Bose gases and Bose-Einstein condensates

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Bose-Einstein Condensation

A large number of (bosonic) atoms, confined to a trap, is cooled to very low temperatures. Below a critical temperature, a large percentage of particles condensate into the same QM one-particle state.

In 1924/25, Bose-Einstein Condensation (BEC) was first predicted by Bose and Einstein from considerations of the non-interacting Bose gas.

In 1995, BEC was first verified experimentally in cold atomic gases (Physics Nobel Prize for Cornell, Wiemann and Ketterle in 2001).

Rich interaction between manybody and nonlinear dispersive effects.

Dilute Bose gas: N bosons in Gross-Pitaevskii scaling

N-particle Schrödinger equation, $\Psi_N(t; x_1, \dots, x_N) \in L^2_{sym}(\mathbb{R}^{dN})$

$$i\partial_t \Psi_N \;=\; H_N \, \Psi_N \quad , \quad \Psi_N(t=0) \;=\; \Psi_{N,0}$$

$$H_N \;:=\; \sum_{j=1}^{N} (-\Delta_{x_j}) \;+\; \sum_{\ell=1}^{N} W_{trap}(x_\ell) \;+\; \frac{1}{N} \sum_{1 \leq i < j \leq N} V_N(x_i - x_j) \, ,$$

$$V_N(x) = N^{d\beta} V(N^\beta x)$$

V sufficiently regular, $0 \leq \beta \leq 1$.

Define the **N-particle density matrix**

$$\gamma_N(t,\underline{x}_N;\underline{x}'_N) \;=\; \Psi_N(t,\underline{x}_N)\overline{\Psi_N(t,\underline{x}'_N)}$$

and **k-particle marginals for $k = 1,\dots,N$,**

$$\gamma_N^{(k)}(t,\underline{x}_k;\underline{x}'_k) \;=\; \int d\underline{x}_{N-k}\gamma_N(t,\underline{x}_k,\underline{x}_{N-k};\underline{x}'_k,\underline{x}_{N-k})\,,$$

where $\underline{x}_k := (x_1,\dots,x_k)$, $\underline{x}_{N-k} := (x_{k+1},\dots,x_N)$.

They are *positive definite* and *admissible*:

$$\gamma_N^{(k)} \;=\; \mathrm{Tr}_{k+1}\gamma_N^{(k+1)} \;\geq\; 0$$

Proof of Bose-Einstein condensation, ground states

[Lieb-Seiringer-Yngvason; Aizenman-L-S-Solovej-Y], [Lewin-Nam-Rougerie],...

$$\Phi_N \text{ ground state of } H_N$$

Then, the 1-particle marginal converges to a rank 1 projection as $N \to \infty$,

$$\gamma^{(1)}_{\Phi_N} \to |\phi\rangle\langle\phi|$$

where ϕ minimizes the GP functional

$$\mathcal{E}[\phi] = \int \Big(\frac{1}{2}|\nabla\phi|^2 + W_{trap}|\phi|^2 + \frac{1}{4}|\phi|^4\Big) \ , \ \ \|\phi\|_{L^2} = 1$$

Thus, 100% of all bosons are in the state ϕ, BEC in the ground state.

What about the dynamics of the BEC ?

Rigorous derivation of mean field equations

The dynamics of a Bose-Einstein Condensate (BEC) is described by a NLS

$$i\partial_t \phi = -\Delta\phi + |\phi|^2\phi$$

or a Hartree equation

$$i\partial_t \phi = -\Delta\phi + (V * |\phi|^2)\phi$$

derived in limit of particle number $N \to \infty$, in Gross-Pitaevskii scaling.

- Via Fock space: *Hepp, Ginibre-Velo, Rodnianski-Schlein, Grillakis-Machedon-Margetis, Grillakis-Machedon*
- Via BBGKY & resolvent estimates: *Spohn, Erdös-Schlein-Yau, Elgart-E-S-Y, Adami-Bardos-Golse-Teta*. Classical case: *Lanford*
- Via BBGKY & nonlinear dispersive PDE: *Klainerman-Machedon, Kirkpatrick-Schlein-Staffilani, C-Pavlović, X.Chen, X.C.-Holmer, C-Hainzl-Pavlović-Seiringer (using Quantum de Finetti)*
- *Fröhlich-Graffi-Schwarz, Fröhlich-Knowles-Pizzo, Anapolitanos-Sigal, Pickl*

Approach via BBGKY hierarchy , [Spohn], [Erdös-Schlein-Yau]

$$i\partial_t \gamma_N^{(k)}(t, \underline{x}_k; \underline{x}'_k) = -\sum_{j=1}^{k} (\Delta_{x_j} - \Delta_{x'_j}) \gamma_N^{(k)}(t, \underline{x}_k; \underline{x}'_k)$$

$$+ \quad \frac{1}{N} \sum_{1 \le i < j \le k} \quad \Big(V_N(x_i - x_j) - V_N(x'_i - x'_j) \Big) \, \gamma_N^{(k)}(t, \underline{x}_k; \underline{x}'_k)$$

$$+ \quad \frac{N-k}{N} \sum_{j=1}^{k} \int \Big(V_N(x_j - y) - V_N(x'_j - y) \Big) \, \gamma_N^{(k+1)}(t, \underline{x}_k, y; \underline{x}'_k, y) dy$$

[ESY] Weak-* convergence as $N \to \infty$ to **GP hierarchy**:

$$i\partial_t \gamma_\infty^{(k)} = -\sum_{j=1}^{k} (\Delta_{x_j} - \Delta_{x'_j})\, \gamma_\infty^{(k)}$$

$$+ \mu \sum_{j=1}^{k} \underbrace{\Big(\gamma_\infty^{(k+1)}(t, x_1, \ldots, x_j, \ldots, x_k, x_j; x'_1, \ldots, x'_k, x_j) - \gamma_\infty^{(k+1)}(t, x_1, \ldots, x_k, x'_j; x'_1, \ldots, x'_j, \ldots, x'_k, x'_j) \Big)}_{=: B_{j;k+1}\gamma^{(k+1)}},$$

for $V_N(x) \rightharpoonup \pm\delta(x)$ when $0 < \beta < 1$ (case $\beta = 1$ much harder)

Derivation of NLS

The GP hierarchy preserves factorization of solutions: Given

$$\gamma_\infty^{(k)}(0) \;=\; \prod_{j=1}^{k} \phi_0(x_j)\,\overline{\phi_0(x_j')} \;\;\Longrightarrow\;\; \gamma_\infty^{(k)}(t) \;=\; \prod_{j=1}^{k} \phi(t,x_j)\,\overline{\phi(t,x_j')}$$

where ϕ solves the cubic NLS

$$i\partial_t\phi \;=\; -\Delta_x\phi \;+\; \mu\,|\phi|^2\,\phi \;\;,\;\; \phi_0 \in L^2(\mathbb{R}^d)$$

Uniqueness of solutions to GP hierarchy in solution space $\mathfrak{H}^1$:

$$\mathrm{Tr}(\,|S^{(k,1)}\gamma^{(k)}|\,) \;<\; C^k \quad , \quad S^{(k,\alpha)} := \prod_{j=1}^{k}\langle\nabla_{x_j}\rangle^{\alpha}\langle\nabla_{x_j'}\rangle^{\alpha}$$

Very hard problem (high dimensional singular integrals, Feynman graph expansions, graph combinatorics).

[ESY], [KM], [CP], [CHPS], ...

Dynamics of fluctuations

- Fock space approach, subleading order in N, used to improve convergence rate in the analysis of Hepp and Rodnianski-Schlein: *Grillakis-Margetis-Machedon, Grillakis-Machedon*.
- Fock space approach, central limit theorem: *Ben Arous-Kirkpatrick-Schlein*
- Quasifree reduction: *Bach-Breteaux-C-Fröhlich-Sigal*.

QFT: Description of a field of indistinguishable quantum particles

Wave function for one particle: $f \in L^2(\mathbb{R}^3)$

Wave function for two indistinguishable particles (bosons):

$$\frac{1}{2}\left(f_1 \otimes f_2 + f_2 \otimes f_1 \right)(x_1, x_2) \in \mathrm{Sym}_2(L^2(\mathbb{R}^3))^{\otimes 2}$$

n indistinguishable particles:

$$\underbrace{\frac{1}{n!}\sum_{\pi \in S_n}}_{\mathrm{Sym}_n} \left(f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)} \right)(x_1, \ldots, x_n) \in \mathfrak{F}_n = \mathrm{Sym}_n(L^2(\mathbb{R}^3))^{\otimes n}$$

Describe states with fluctuating particle # by vectors in boson Fock space

$$\mathfrak{F} \;=\; \bigoplus_{n\geq 0} \mathfrak{F}_n$$

Zero particle space: $\mathfrak{F}_0 \;=\; \mathbb{C}$. Vacuum vector $\Omega = (1, 0, 0, \dots)$.

Introduce creation and annihilation operators

$$\psi^*(f) \quad = \quad \mathrm{Sym}_{n+1} f \otimes \bullet \qquad : \; \mathfrak{F}_n \to \mathfrak{F}_{n+1}$$

$$\psi(f) \quad = \quad \big\langle\, f \,,\, \bullet \,\big\rangle_{L^2_{x_n}(\mathbb{R}^3)} \qquad : \; \mathfrak{F}_n \to \mathfrak{F}_{n-1}$$

under the condition that

$$\psi(f)\,\Omega \;=\; 0 \qquad \forall\, f \in L^2(\mathbb{R}^3)$$

Then, n bosons with wave functions $f_1, \ldots, f_n \in L^2(\mathbb{R}^3)$:

$$\Phi^{(n)} \;=\; \psi^*(f_1) \cdots \psi^*(f_n)\,\Omega \;=\; \mathrm{Sym}_n\, f_1 \otimes \cdots \otimes f_n \;\in\; \mathfrak{F}_n$$

Linear span of such states, for $n \geq 0$, is dense in $\mathfrak{F}$.

$$\Phi \;=\; (\Phi^{(0)}, \Phi^{(1)}, \ldots, \Phi^{(n)}, \ldots) \;\in\; \mathfrak{F}$$

Inner product: $\big\langle \Phi, \Psi \big\rangle_{\mathfrak{F}} \;=\; \sum_n \big\langle \Phi^{(n)}, \Psi^{(n)} \big\rangle_{\mathfrak{F}_n}$

Adjoints $\psi^*(f) = (\psi(f))^*$. Canonical commutation relations

$$[\psi(f), \psi^*(g)] \;=\; \big\langle f, g \big\rangle_{L^2} \quad , \quad [\psi^\sharp(f), \psi^\sharp(g)] \;=\; 0$$

$\psi^*(f)$, $\psi(f)$ are linear/antilinear in $f \in L^2(\mathbb{R}^3)$. Can write

$$\psi(f) \quad = \quad \int dx\, f^*(x)\, \psi(x)$$

$$\psi^*(f) \quad = \quad \int dx\, f(x)\, \psi^*(x) \quad = \quad (a(f))^*$$

Operator-valued distributions $\psi^*(x)$, $\psi(x)$, CCR

$$\begin{aligned} \big[\psi(x), \psi^*(y)\big] &= \delta(x-y) \\ \big[\psi(x), \psi(y)\big] &= 0 = \big[\psi^*(x), \psi^*(y)\big]\,. \end{aligned}$$

Fock vacuum $\Omega \in \mathcal{F}$, with $\psi(x)\Omega = 0\ \forall x \in \mathbb{R}^3$.

Operators acting on $\mathfrak{F}$ = *observables*

Boson Hamiltonian

$$\mathbb{H} = \int dx\; \psi^*(x)(-\Delta\psi)(x) + \frac{1}{2}\int dxdy\; \psi^*(x)\psi(x)v(x-y)\psi^*(y)\psi(y),$$

Interaction pot. $v(x) = v(-x)$, with $v^2 \leq C(1-\Delta)$. $\mathbb{H}$ selfadjoint on $\mathcal{F}$.

$\mathbb{H}$ acts on $\Phi \in \mathcal{F}$ as

$$\Big(\mathbb{H}\Phi\Big)^{(n)} = \Big(\sum_{j=1}^{n}(-\Delta_{x_j}) + \sum_{1\leq i<j\leq n} V_N(x_i - x_j)\Big)\Phi^{(n)} \tag{1}$$

Quantum states

$\mathfrak{A}$ the C^* algebra of observables $\mathbb{A}$ (norm closure of bounded lin ops on $\mathfrak{F}$).

$\mathfrak{S} = \{$ normalized, positive semidefinite states $\}$

$= \{$ linear functionals $\omega : \mathfrak{A} \to \mathbb{C}$ satisfying $\omega(\mathbf{1}) = 1$, $\omega(\mathbb{A}^*\mathbb{A}) \geq 0$ and

$\omega(\mathbb{A}^*) = \overline{\omega(\mathbb{A})}$ for all $\mathbb{A} \in \mathfrak{A}$ $\}$

Example: $\omega(\mathbb{A}) = \mathrm{Tr}(\rho\mathbb{A})$ for some trace class operator ρ with $\mathrm{Tr}\rho = 1$.

Evolution of states is determined by the von Neumann-Landau equation

$$i\partial_t \omega_t(\mathbb{A}) = \omega_t([\mathbb{A}, \mathbb{H}]) \quad , \quad \forall \text{ observables } \mathbb{A}$$

Solution is given by

$$\omega_t(\mathbb{A}) = \omega_0(e^{-it\mathbb{H}}\mathbb{A}e^{it\mathbb{H}})$$

Quasifree states

Truncated expectations: Abbreviate $\psi_j := \psi^{\sharp_j}(x_j)$.

n^{th} order *truncated expectations (correlations)* $\omega^T(\psi_1, \ldots, \psi_n)$ of a state ω are defined recursively via

$$\omega(\psi_1 \cdots \psi_n) = \sum_{P_n} \prod_{J \in P_n} \omega^T(\psi_{i_1}, \ldots, \psi_{i_{\#(J)}})$$

P_n partitions of the ordered set $\{1, ..., n\}$ into ordered subsets, J.

For example

$$\begin{aligned} \omega^T(\psi(x)) &= \omega(\psi(x)), \\ \omega^T(\psi_1, \psi_2) &= \omega(\psi_1 \psi_2) - \omega(\psi_1)\,\omega(\psi_2). \end{aligned}$$

A state ω is *quasifree* if

$$\omega^T(\psi_1, \ldots, \psi_n) = 0 \ \ \forall\, n > 2$$

Denote space of quasifree states $\mathfrak{Q} = \{\omega^q \text{ quasifree}\}$.

Quasifree reduction and HFB equations

[V. Bach, S. Bretaux, T.C., J. Fröhlich, I.M Sigal 2016]

For quasifree states, all expectations of order > 2, can be expressed through the 1st and 2nd order truncated expectations.

Quasifree reduction of ω_t: Given quasifree initial state $\omega_0 \in \mathfrak{Q}$, find family $(\omega_t^q)_{t\geq 0} \in C^1\left(\mathbb{R}_0^+; \mathfrak{Q}\right)$ of quasifree states satisfying

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]) \tag{2}$$

for all observables $\mathbb{A}$ *at most quadratic in* ψ, ψ^*.

ω^q determines and is determined by the truncated expectations to order 2:

$$\begin{cases} \phi(x) := \omega^q(\psi(x)), \\ \gamma(x;y) := \omega^q[\psi^*(y)\,\psi(x)] - \omega^q[\psi^*(y)]\,\omega^q[\psi(x)], \\ \sigma(x,y) := \omega^q[\psi(x)\,\psi(y)] - \omega^q[\psi(x)]\,\omega^q[\psi(y)]\,. \end{cases} \tag{3}$$

This definition implies that

$$\gamma = \gamma^* \geq 0 \;\text{ and }\; \sigma^* = \bar{\sigma}, \tag{4}$$

where $\bar{\sigma} = C\sigma C$ with C being the complex conjugation.

Evaluating (2) for monomials $\mathbb{A} \in \mathcal{A}^{(2)}$, where

$$\mathcal{A}^{(2)} := \{\psi(x), \psi^*(x)\psi(y), \psi(x)\psi(y)\},$$

yields equivalent system of coupled nonlinear PDE's for $(\phi_t, \gamma_t, \sigma_t)$, the *Hartree-Fock-Bogoliubov (HFB) equations*.

Physical interpretation:

ϕ_t wave function for the Bose-Einstein condensate,

γ_t and σ_t dynamics of sound waves in the quasifree approximation.

Emission, reabsorption of 1, resp. 2 particles from BEC into thermal cloud.

The HFB equations provide a *time-dependent extension* of the standard stationary Hartree-Fock-Bogoliubov equations for a Bose gas appearing in the physics literature.

Rem: [Grillakis-Machedon] derive HFB equations for special case where $\gamma_t = \cosh(2k_t)$, $\sigma_t = \sinh(2k_t)$ are pure states, determined by a single kernel k_t.

Main Results

Thm

Let $[A_1, A_2]_\pm := A_1 A_2^T \pm A_2 A_1^T$, and define

$$\gamma^\phi := \gamma + |\phi\rangle\langle\phi| \ \ , \ \ \sigma^\phi := \sigma + \phi \otimes \phi \,,$$

(acting as integral operators), and

$$h_v(\gamma) := -\Delta + b[\gamma] \quad , \quad b[\gamma] := v * n_\gamma + v \,\#\, \gamma \,,$$
$$(v\#\sigma)(x,y) := v(x-y)\sigma(x,y) \quad , \quad n_\gamma(x) := \gamma(x,x).$$

Then, the quasifree state $\omega_t^q \in \mathcal{X}_{T,\mathrm{qf}}^\infty$ satisfies

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]) \ , \ \ \forall\, \mathbb{A} \in \mathcal{A}^{(2)} \,,$$

iff $(\phi_t, \gamma_t, \sigma_t) \in \mathcal{X}_T^\infty$ associated to ω_t^q satisfies the time-dependent HFB eqs

$$\begin{aligned}
i\partial_t \phi_t &= h_v(\gamma_t)\phi_t \ + \ (v\#\sigma_t^{\phi_t})\bar{\phi}_t \,, \\
i\partial_t \gamma_t &= [h_v(\gamma_t^{\phi_t}), \gamma_t]_- \ + \ (v\#\sigma_t^{\phi_t})\sigma_t^* \ - \ \sigma_t(v\#\sigma_t^{\phi_t})^* \,, \\
i\partial_t \sigma_t &= [h_v(\gamma_t^{\phi_t}), \sigma_t]_+ + [(v\#\sigma_t^{\phi_t}), \gamma_t]_+ \ + \ v\#\sigma_t^{\phi_t},
\end{aligned}$$

Def

Given ω^q quasifree, (ϕ, γ, σ) defines the quadratic HFB Hamiltonian

$$\begin{aligned}\mathbb{H}_{HFB}(\omega^q) = &\int \psi^*(x) h_v(\gamma)\psi(x)\, dx \\ &- \int b[|\phi\rangle\langle\phi|]\phi(x)\psi^*(x)\, dx + h.c. \\ &+ \frac{1}{2}\int \psi^*(x)(v\#\sigma)\psi^*(x)\, dx + h.c.\end{aligned} \tag{5}$$

Thm

The triple $(\phi_t, \gamma_t, \sigma_t)$ satisfies the HFB equations iff the corresponding quasifree state ω_t^q satisfies

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}_{HFB}(\omega_t^q)]) \quad \forall \mathbb{A} \in \mathfrak{A}\,. \tag{6}$$

Conservation laws for the quasifree dynamics

Observables quadratic in ψ, ψ^* that are conserved for the full dynamics are also conserved for the quasifree dynamics.

Thm

Assume that the observable $\mathbb{A} \in \mathcal{A}^{(2)}$ satisfies $[\mathbb{H}, \mathbb{A}] = 0$.
Then, $\omega_t^q(\mathbb{A})$ is conserved:

$$\omega_t^q(\mathbb{A}) \;=\; \omega_0^q(\mathbb{A}) \quad \forall\, t \in \mathbb{R}\,. \tag{7}$$

Proof. Since

$$i\partial_t \omega_t^q(\mathbb{A}) \quad = \quad \omega_t^q([\mathbb{A}, \mathbb{H}])\;, \;\; \forall\, \mathbb{A} \in \mathcal{A}^{(2)}\,,$$

the statement follows immediately. □

Cor

Let $\omega_t^q \in \mathcal{X}_T^{\mathrm{qf}}$ solve

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}_{HFB}(\omega_t^q)])\,.$$

Then, the particle number

$$\mathcal{N}(\phi_t, \gamma_t, \sigma_t) = \omega_t^q(\mathbb{N}) \;=\; \int \big(\gamma(x;x) + |\phi(x)|^2\big)dx$$

and the HFB energy are conserved,

$$\begin{aligned}\mathcal{E}(\phi, \gamma, \sigma) = \omega_t^q(\mathbb{H}) = \mathrm{Tr}[h(\gamma + |\phi\rangle\langle\phi|)] + \mathrm{Tr}[b[|\phi\rangle\langle\phi|]\gamma] \\ + \frac{1}{2}\mathrm{Tr}[b[\gamma]\gamma] + \frac{1}{2}\int v(x-y)|\sigma(x,y) + \phi(x)\phi(y)|^2 dxdy\,.\end{aligned}$$

from $i\partial_t \omega_t^q(\mathbb{H}) = \omega_t^q([\mathbb{H}, \mathbb{H}_{HFB}(\omega_t^q)]) = \omega^q([\mathbb{H}_{HFB}(\omega_t^q), \mathbb{H}_{HFB}(\omega_t^q)]) = 0$

Global well-posedness for HFB equations

Def

X a Banach space, $f \in C(X)$ continuous on X, $G(t)$ a strongly continuous semigroup with infinitesimal generator $-iA$.

$\rho \in C([0,T), X)$ is a *mild solution* of the Cauchy problem

$$\begin{cases} i\partial_t \rho & = A\rho + f(\rho)\,, \\ \rho(0) & = \rho_0 \in X\,, \end{cases}$$

if ρ_t solves the fixed point equation in integral form

$$\rho_t = G(t)\rho_0 - i\int_0^t G(t-s)f(\rho_s)\,ds$$

Our space of solutions will be $X = X^1$,

$$\|(\phi,\gamma,\sigma)\|_{X^1} = \|\langle\nabla\rangle\phi\|_{L^2(\mathbb{R}^d)} + \|\langle\nabla\rangle\gamma\langle\nabla\rangle\|_{\mathcal{L}^1} + \|(\langle\nabla\rangle^2\otimes 1 + 1\otimes\langle\nabla\rangle^2)^{1/2}\sigma\|_{L^2(\mathbb{R}^{2d})}.$$

Thm

Let $d \leq 3$ and $\rho_0 = (\phi_0, \gamma_0, \sigma_0) \in X^1$, and $V = 0$, v sufficiently regular.

Then the following hold:

1. *Existence and uniqueness of a local mild solution:*

   There exists a unique local mild solution

   $$(\rho_t)_{t\in[0,T)} = (\phi_t, \gamma_t, \sigma_t)_{t\in[0,T)} \in C^0([0,T); X^1)$$

   to the HBF equations for the given initial data, for some $0 < T \leq \infty$.

2. *Conservation laws:*

   The particle number and the HFB energy are conserved.

3. *Existence of a global solution:*

   If also $\Gamma_0 = \begin{pmatrix} \gamma_0 & \sigma_0 \\ \bar{\sigma}_0 & 1 + \bar{\gamma}_0 \end{pmatrix} \geq 0$, the solution is global, $T = \infty$.

Gibbs states and BEC

Put system on torus $\Lambda_L = [-L, L]^d$ with periodic boundary conditions.

$\Lambda_L^* := \frac{\pi}{L}\mathbb{Z}^d$ lattice reciprocal to Λ_L.

Let $V = 0$ (external potential).

We will eventually take the thermodynamic limit, $L \to \infty$, and discuss the emergence of a Bose-Einstein condensate.

The Hamiltonian $\mathbb{H}$ of the Bose gas is **translation invariant** and $U(1)$ **gauge-invariant**: Invariant under transformation $\psi^\sharp \to (e^{i\theta}\psi)^\sharp$.

On compact torus, where the volume is finite, **these symmetries are also present in the Gibbs states of system**.

We want to determine quasifree Gibbs states ω_L^q which satisfy:

• Both the $U(1)$ gauge invariance and the translation invariance,

• The fixed point equation corresponding to the self-consistency condition

$$\begin{aligned} \Phi_{\omega_L^q}(\mathbb{A}) &:= \frac{1}{\Xi}\mathrm{Tr}\Big[\mathbb{A}\ \exp(-\beta(\mathbb{H}_{HFB}(\omega_L^q) - \mu\mathbb{N}))\Big] \\ \Xi &= \mathrm{Tr}\Big[\exp(-\beta(\mathbb{H}_{HFB}(\omega_L^q)) - \mu\mathbb{N})\Big] \\ \Phi_{\omega_L^q} &= \omega_L^q \end{aligned} \tag{8}$$

with inverse temperature $\beta > 0$ and chemical potential μ.

The $U(1)$ gauge-invariance of ω_L^q implies $\phi_{\omega_L^q} = 0$ and $\sigma_{\omega_L^q} = 0$: Indeed, $\omega^q(\psi) = \omega^q(e^{i\theta}\psi) = e^{i\theta}\omega^q(\psi)$, hence $\phi_{\omega^q} = 0$. Similarly, $\sigma_{\omega^q} = 0$.

These quasifree states are thus characterized only by γ_L, hence we may replace ω_L^q by γ_L in the sequel.

For quasifree, $U(1)$-gauge invariant states, the HFB equations reduce to the bosonic Hartree-Fock equation.

Related work of [Napiorkowski-Reuvers-Solovej]:

For $V = 0$ and γ and σ translationally invariant, our HFB energy functional reduces to the energy density functional considered in [N-R-S].

[N-R-S] prove that this functional has $U(1)$ gauge symmetry breaking minimizers ($\phi \neq 0$) of the Bogoliubov free energy, and the appearance of BEC for the corresponding minimizers.

(But one still has to show that states thus obtained are stationary solutions to the dynamical HFB equations.)

Let $v = g\delta$ for simplicity.

By translation invariance, $\gamma_L(x;y)$ is a function of $x - y$, thus $n = n(x) = \gamma_L(x;x)$ is independent of x.

The HFB Hamiltonian then reduces to

$$\mathbb{H}_{HFB}(\omega_L^q) = \int dx\, \psi^*(x)\, ((-\Delta + gn)\psi)(x)\,, \tag{9}$$

with $n = n(x) = \gamma_L(x;x)$.

Applying the fixed point equation (8) with $\mathbb{A} = \psi^*(y)\psi(x)$ yields

$$\gamma_L = \frac{1}{\exp(\,\beta(\,-\Delta + gn\mathbf{1} - \mu\mathbf{1})\,)\; - \;\mathbf{1}}\,, \tag{10}$$

for $n \in [0, \infty)$. γ_L is a pseudodifferential operator with symbol

$$\hat{\gamma}_L(k) := \int_{\Lambda_L} \gamma_L(x) e^{-ix\cdot k} dx = \frac{1}{\exp(\beta(k^2 + gn - \mu)) - \mathbf{1}} \tag{11}$$

Thus

$$n = \gamma_L(0) = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k)\,. \tag{12}$$

We thus obtain a *nonlinear fixed point equation* for n:

$$n = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{1}{\exp(\beta(k^2 + gn - \mu)) - 1}\,. \tag{13}$$

Let $g, \beta, n > 0$, and $d \geq 3$.

Define, for given $\beta > 0$ and $g > 0$, the critical chemical potential

$$\mu_c = \mu_c(\beta, g) := g \int \frac{dk}{e^{\beta k^2} - 1}\,, \tag{14}$$

which is finite in dimension $d = 3$ (or higher).

Thm

The case $\mu < \mu_c$: The fixed point equation

$$n = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^* \setminus \{0\}} \frac{1}{e^{\beta(k^2+gn-\mu)} - 1} = \int \frac{dk}{e^{\beta(k^2+gn-\mu)} - 1} \tag{15}$$

has a unique solution $n_* = n_*(\beta, \mu, g)$ which satisfies $gn_* - \mu > 0$.

In the HFB Gibbs state parametrized with (β, μ), we obtain

$$\gamma(x, y) = \int \frac{e^{2\pi ik(x-y)}}{e^{\beta k^2+gn_*-\mu} - 1} dk\,. \tag{16}$$

In this case, no Bose-Einstein condensation occurs.

Proof. For fixed n, the thermodynamic limit

$$\begin{aligned} \mathcal{M}(n) &:= \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{k\in\Lambda_L^*\setminus\{0\}} \frac{1}{e^{\beta(k^2+gn-\mu)}-1} \\ &= \int \frac{dk}{e^{\beta(k^2+gn-\mu)}-1} \end{aligned} \tag{17}$$

is well defined. Goal is to find a solution to the fixed point equation

$$n = \mathcal{M}(n) \tag{18}$$

with

$$\nu := gn - \mu \geq 0 \tag{19}$$

(if $gn - \mu < 0$, the integral diverges, and no equilibrium state exists).

Rewrite into a fixed point equation for $\nu \geq 0$, using $n = \frac{\mu+\nu}{g}$,

$$\frac{\mu}{g} + \frac{\nu}{g} = \int \frac{dk}{e^{\beta(k^2+\nu)} - 1} =: G(\nu)\,. \tag{20}$$

$G(\nu)$ strictly monotonically decreasing in ν, with max at $G(0) = \frac{\mu_c}{g}$.

L.h.s. linear, strictly monotonically increasing ν for any $g > 0$.

Thus, the graphs of the left and of the right hand side of (20) intersect at precisely one point, $\nu_* = \nu_*(\beta, \mu, g) > 0$.

We then find that $n_* = n_*(\beta, \mu, g)$, defined by

$$n_* := \frac{\mu + \nu_*}{g} = \int \frac{dk}{e^{\beta(k^2+gn_*-\mu)} - 1}\,, \tag{21}$$

solves the desired fixed point equation. □

Thm

The case $\mu \geq \mu_c = \mu_c(\beta, g)$. Define the BEC density by

$$\rho_{BEC} = \frac{\mu - \mu_c}{g} \geq 0\,. \tag{22}$$

Then, in the HFB Gibbs state parametrized with (β, μ), the two-point function is given by

$$\gamma(x, y) = \rho_{BEC} + \int \frac{e^{2\pi i k(x-y)}}{e^{\beta k^2} - 1} dk\,. \tag{23}$$

In particular, the total density of the system is given by

$$n_* = \gamma(x, x) = \frac{\mu}{g}\,, \tag{24}$$

so that

$$g n_* - \mu = 0 \tag{25}$$

holds. Thus, Bose-Einstein condensation occurs whenever $\mu > \mu_c$.

Proof. Goal is to find equilibrium state of HFB system with $gn_* - \mu = 0$ (divergence if < 0). Given $gn_* - \mu = 0$,

$$\kappa(k) := \frac{1}{e^{\beta(k^2+gn-\mu)} - 1} = \frac{1}{e^{\beta k^2} - 1} \,. \tag{26}$$

Thus, in the thermodynamic limit,

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{|k|>0} \kappa(k) = \int_{\mathbb{R}^3} \kappa(k) dk = \frac{\mu_c}{g} \,. \tag{27}$$

From translation invariance,

$$\gamma(x, y) = \int K_\gamma(k) e^{2\pi i k(x-y)}\, dk \tag{28}$$

where for $|k| > 0$, $K_\gamma(k) = \kappa(k)$.

Since $\kappa(k)$ diverges in the limit $|k| \to 0$, allow for a delta measure $M\delta$ concentrated at $|k| = 0$ in thermodynamic limit,

$$K_\gamma(k) = M\delta(k) + \frac{1}{e^{\beta k^2} - 1} \,. \tag{29}$$

The density $n = \frac{\mu}{g}$ is related to M via

$$\begin{aligned} n_* = \frac{\mu}{g} &= M + \int \nu(k)dk \\ &= M + \frac{\mu_c}{g} \, . \end{aligned} \tag{30}$$

Therefore, we find that if the chemical potential satisfies $\mu \geq \mu_c$,

$$\rho_{BEC} = M = \frac{\mu - \mu_c}{g} \geq 0 \tag{31}$$

is the density of the Bose-Einstein condensate. □

Thank you for your attention !