MEAN-FIELD LIMITS FOR QUANTUM SYSTEMS AND NONLINEAR GIBBS MEASURES

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ABSTRACT

We consider the linear Schrödinger equation describing N quantum (bosonic) particles at equilibrium and study its behavior as N tends to infinity. We place the system in the mean-field regime, in which the particles are very tightly packed but interact weakly. In this limit we prove that they become essentially independent and identically distributed according to a nonlinear partial differential equation. Our main tool is the quantum de Finetti theorem, an abstract result about how independence can arise due to symmetry in such systems. By considerably increasing the randomness in the system, we can also obtain nonlinear Gibbs measures. Those are probability measures over an infinite-dimensional space, which play a major role in different areas of mathematics. The two- and three-dimensional cases are particularly challenging due to the necessity of using a renormalization procedure to cancel infinities.

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1. INTRODUCTION

Mathematics is efficient in describing some aspects of our world [63]. Many complicated natural phenomena are well reproduced using rather simple equations. More than that, abstract results or principles can sometimes even be used to *predict* new phenomena, later confirmed by experiments. This happened many times in physics in the 20th century, in particular through *arguments based on symmetry*. Several elementary particles were discovered this way (such as the positron predicted by Dirac in 1928 and discovered later by Anderson in 1932 or, more recently, the Higgs boson). In this respect, mathematics is not just an efficient tool to model our world, it can sometimes also be used to explore it.

Quantum mechanics is certainly one of the physical theories relying the most on mathematics. This is in part due to the strong influence of Hilbert in Göttingen, where Heisenberg and Born invented the "new quantum mechanics" around 1925 [56, 58]. In fact, several mathematical concepts used all the time today (such as the Hilbert space) have been invented in this context [62]. This is a culmination of Hilbert's program to axiomatize physics, his 6th problem at the International Congress of Mathematics in 1900 [31].

At about the same time that quantum mechanics was being formalized, Bose [10] and Einstein [19] predicted the existence of a new state of matter, now called a *Bose–Einstein condensate*. Their argument was again mainly based on symmetry. Under the assumption that the wave function of a set of N particles is invariant under the action of the permutation group $\mathfrak{S}_N$, they found that those particles would have to behave rather strangely when N gets large, at very low temperatures. When the temperature passes below some critical value, they start traveling through the whole system at macroscopic distances, and all adopt the exact same behavior on average. A condensate is thus a macroscopic piece of quantum matter, where quantum effects can almost be observed with the human eye. The particles respecting this symmetry are now called *bosons*; famous examples include photons and helium atoms. Even if Bose–Einstein condensation (BEC) was suspected to play a role in many experiments (e.g., for the superfluidity of liquid helium), it was only in 1995 that a condensate could finally be realized in the laboratory [4, 13]. This was recognized by a Nobel prize in 2001 and is still a very active subject of research in theoretical and experimental physics.

The argument of Bose and Einstein concerned noninteracting particles, and it can be made rigorous. However, real particles interact with each other and providing a mathematical proof of condensation in this case turned out to be very difficult, even at zero temperature. This was finally achieved in a series of works by Lieb, Seiringer, and Yngvason [43–46, 50] starting in 1998. These works belong to a large trend of research in analysis and mathematical physics which was stimulated by the numerous experimental discoveries starting from 1995.

In this paper I present the results obtained on the subject with my collaborators in the four articles [37, 38, 41, 42] published in the period 2014–2021. In [37] we realized with Phan Thành Nam and Nicolas Rougerie that BEC can, to some extent, be understood through a purely abstract result, the *quantum de Finetti theorem*. A version of this theorem was proved in 1969 [33, 60] within the framework of operator algebras, and it currently plays an important role in quantum information theory. Its use for the condensation of bosons had, however,

been rather anecdotal. The *classical* version of de Finetti's theorem dates back to 1931 and is often called the *Hewitt–Savage theorem* [14, 30]. It plays a central role in probability and statistics. Loosely speaking, the latter says that a sequence of infinitely many *exchangeable random variables* is essentially automatically independent and identically distributed (i.i.d.). More precisely, its law must be the convex combination of i.i.d. random variables. Similarly, we will see that the emergent macroscopic i.i.d. behavior of the bosons in a condensate is a consequence of their indistinguishability, which implies a certain symmetry under permutations.

This point of view allowed us to push forward the mathematical analysis of condensates. In particular, in [38, 41] we started to look at a new situation where the randomness between the condensed particles is considerably increased, due to the temperature. This corresponded to looking at how the condensate is forming, just before the phase transition. We showed that the condensed bosons are then described by *nonlinear Gibbs measures*. These probability measures in infinite dimension play a major role in several areas of mathematics. They, for instance, appear in the study of rough stochastic partial differential equations and of deterministic equations with random initial data (as promoted by Bourgain [11, 12] and now studied by many authors). Our new program has generated some interest and important achievements followed, in particular by Fröhlich, Knowles, Schlein, and Sohinger [22–24].

We shall restrict here our attention to a particular regime, called the *mean-field limit*. The system is assumed to be very dense (hence the particles meet very often) but the particles interact only a little. The many-particle interaction then gets replaced by an *effective nonlinear interaction*, seen by all the particles in the system, which leads to a nonlinear partial differential equation. This is not the most common regime in experiments [4, 13]. The system is often rather dilute such that the particles instead meet rarely. The Lieb–Seiringer–Yngvason analysis in this case is more involved and requires more assumptions [43–46, 50].

In the next section we introduce the Schrödinger model for N bosons. In Section 3 we review our main results on Bose–Einstein condensation in the mean-field limit from [37, 42]. We then turn in Section 4 to a different mean-field regime where nonlinear Gibbs measures appear [38, 41]. Due to space limitations, we will avoid entering too much into the technical details. We will also not be able to cite all the existing literature. In addition to [37, 38, 41, 42], we refer to a previous proceedings [36] for more references (in particular on the physics side), and to [57] for a recent and detailed review of known results.

2. THE N-PARTICLE QUANTUM MODEL

We consider a system composed of N identical particles evolving in $\mathbb{R}^d$. Physically $d \in \{1, 2, 3\}$, but for the moment any $d \geq 1$ is allowed. We assume that interactions take place by pairs and are described with an even potential $w : \mathbb{R}^d \to \mathbb{R}$. We ignore more complicated events involving three or more particles at a time. We also submit our system to an external potential $V : \mathbb{R}^d \to \mathbb{R}$, which is typically used to ensure that the particles do not escape.

In classical mechanics, our particles would be described by N vectors $\{(x_j, p_j)\}_{j=1}^N$ in $\mathbb{R}^d \times \mathbb{R}^d$, where x_j is the position of the jth particle and $p_j = mv_j$ is its momentum

(mass times velocity). The time evolution is a Hamiltonian system based on the energy

$$\mathcal{H}_{\mathrm{cl}}(x_1, p_1, \dots, x_N, p_N) = \sum_{j=1}^{N} \frac{|p_j|^2}{2m} + \sum_{j=1}^{N} V(x_j) + \lambda \sum_{1 \leqslant j < k \leqslant N} w(x_j - x_k),$$

with the usual symplectic form on the phase space. The three terms are respectively the kinetic energy, the potential energy, and the interaction energy. We have inserted a *coupling constant* λ which we will later use to tune the strength of the interaction between the particles. The usual Hamilton equations lead to Newton's equations that the acceleration is proportional to the forces felt by each particle (which depend on the positions of all the others). Stationary states correspond to critical points of $\mathcal{H}_{\mathrm{cl}}$. Those always have all the p_j equal to 0 (the particles do not move!). Equilibrium states are those where $\mathcal{H}_{\mathrm{cl}}$ is a local minimum. Of interest are also measures on the phase space $(\mathbb{R}^d \times \mathbb{R}^d)^N$ which are globally invariant under the Hamiltonian flow. This is the case of any function of the conserved Hamiltonian $\mathcal{H}_{\mathrm{cl}}$ but an important example is given by the *Gibbs measures*

$$\begin{aligned} \mathcal{P}(x_1, p_1, \dots, x_N, p_N) &= Z^{-1} e^{-T^{-1}\mathcal{H}_{\mathrm{cl}}(x_1, p_1, \dots, x_N, p_N)}, \\ Z &:= \int_{\mathbb{R}^{2dN}} e^{-T^{-1}\mathcal{H}_{\mathrm{cl}}} \mathrm{d}x_1 \cdots \mathrm{d}p_N, \end{aligned} \tag{2.1}$$

where T is a temperature used to model the amount of randomness in the system. In the limit $T \to 0^+$, the probability measure $\mathcal{P}$ concentrates on the minimum of $\mathcal{H}_{\mathrm{cl}}$.

For microscopic particles such as atoms, the classical model is not sufficiently precise and one has to switch to quantum mechanics. The basic principle is to give up the idea that one can know the exact positions and momenta of the particles. Instead, quantum mechanics provides us with two probability measures on $(\mathbb{R}^d)^N$ corresponding to the possible positions and momenta, respectively. These two probability measures are not independent, on account of Heisenberg's uncertainty principle which states that positions and velocities cannot be known simultaneously to an arbitrary precision. This principle is mathematically expressed using the Fourier transform. Namely, our N quantum particles are represented by a square-integrable function $\Psi \in L^2(\mathbb{R}^{dN}, \mathbb{C})$ called the *wave function*, normalized in the manner $\int_{\mathbb{R}^{dN}} |\Psi|^2 = 1$, and it is postulated that

- $|\Psi(x_1, \dots, x_N)|^2$ is the probability density that the particles are at $x_1, \dots, x_N \in \mathbb{R}^d$;
- $|\widehat{\Psi}(p_1, \dots, p_N)|^2$ is the probability density that they have the momenta $p_1, \dots, p_N$.[1]

Integrating the above two probability densities against the classical energy and using that $\widehat{-i\partial_{x_j}\Psi} = p_j \widehat{\Psi}$, we find that the quantum energy can be expressed in terms of Ψ as

$$\mathcal{E}(\Psi) = \frac{1}{2m} \int_{\mathbb{R}^{dN}} |\nabla \Psi|^2 + \sum_{j=1}^{N} \int_{\mathbb{R}^{dN}} V(x_j)|\Psi|^2 + \lambda \sum_{1 \leqslant j < k \leqslant N} \int_{\mathbb{R}^{dN}} w(x_j - x_k)|\Psi|^2. \tag{2.2}$$

1 Here $\widehat{\Psi}(p_1, \dots, p_N) = (2\pi)^{-\frac{dN}{2}} \int_{\mathbb{R}^{dN}} \Psi(x_1, \dots, x_N) e^{-i\sum_{j=1}^{N} x_j \cdot p_j} \mathrm{d}x_1 \cdots \mathrm{d}x_N$.

This is the quadratic form associated with the operator

$$\boxed{H_{N,\lambda} := \sum_{j=1}^{N} \frac{-\Delta_{x_j}}{2m} + \sum_{j=1}^{N} V(x_j) + \lambda \sum_{1 \leq j < k \leq N} w(x_j - x_k)} \tag{2.3}$$

which is our main object of interest. We will work in a system of units so that $2m = 1$.

Since our N particles are all the same, the two probability densities $|\Psi|^2$ and $|\widehat{\Psi}|^2$ must be *symmetric functions*, that is, invariant if we permute their variables. Some additional constraints are thus needed on Ψ. Only two possible choices can preserve the linear character of quantum mechanics, namely Ψ must itself be either symmetric or antisymmetric. This corresponds to the two types of quantum particles existing in Nature, respectively called *bosons* and *fermions*. In this paper we exclusively consider the bosonic case, and hence restrict $H_{N,\lambda}$ to the subspace of symmetric square-integrable functions, denoted by

$$\begin{aligned} &L^2_s\big((\mathbb{R}^d)^N, \mathbb{C}\big) \\ &\quad = \big\{\Psi \in L^2\big((\mathbb{R}^d)^N, \mathbb{C}\big) \,:\, \Psi(x_{\sigma(1)}, \ldots, x_{\sigma(N)}) = \Psi(x_1, \ldots, x_N),\ \forall \sigma \in \mathfrak{S}_N\big\}. \end{aligned}$$

We emphasize that each x_j is in $\mathbb{R}^d$. We are not permuting the coordinates of a given particle.

The quantum model is again a Hamiltonian system, in infinite dimension. Equilibrium states are critical points of the quantum energy $\mathcal{E}$ in (2.2), on the unit sphere of $L^2_s((\mathbb{R}^d)^N, \mathbb{C})$. Those are exactly the symmetric eigenfunctions of the Hamiltonian $H_{N,\lambda}$, which solve Schrödinger's equation

$$H_{N,\lambda}\Psi = E\Psi. \tag{2.4}$$

We will be particularly interested in what is called the *ground state* (the equilibrium state of lowest possible energy), that is, the first eigenfunction. The corresponding energy is

$$\boxed{E(N,\lambda) := \min \sigma(H_{N,\lambda}) = \inf_{\int |\Psi|^2 = 1} \mathcal{E}(\Psi)}$$

where $\sigma(H)$ denotes the spectrum of an operator H. Other states of interest are *quantum Gibbs states*, which are given by a formula similar to the classical case (2.1) by

$$\Gamma_{T,N,\lambda} := Z^{-1}_{T,N,\lambda} e^{-T^{-1}H_{N,\lambda}}, \quad Z_{T,N,\lambda} = \operatorname{Tr}(e^{-T^{-1}H_{N,\lambda}}), \tag{2.5}$$

with the trace taken only over the symmetric subspace $L^2_s((\mathbb{R}^d)^N, \mathbb{C})$. Those are compact operators which involve the whole spectrum of the quantum operator $H_{N,\lambda}$. The corresponding free energy of the system is then given by

$$F(T,N,\lambda) := -T \log Z_{T,N,\lambda} \tag{2.6}$$

and it converges to $E(N,\lambda)$ in the limit $T \to 0^+$. We postpone the presentation of the precise assumptions on the potentials V and w which ensure that this is all well defined.

Finding the equilibrium states (2.4) or the Gibbs state (2.5) requires diagonalizing the operator $H_{N,\lambda}$. Due to the high dimensionality of the problem, this is impossible in most physical situations, even numerically at a sufficiently high precision. It is therefore important to rely on simpler approximations that are both precise enough and suitable to numerical

investigation. One of the most famous is the *mean-field model*, which consists in assuming that the particles are independent but evolve in an effective, self-consistent, potential which replaces the many-particle interaction. The *linear* many-body Schrödinger equation (2.4) on $\mathbb{R}^{dN}$ is then replaced by a more tractable *nonlinear* equation in $\mathbb{R}^d$. Introduced by Curie and Weiss to describe phase transitions in the classical Ising model, the mean-field method is now extremely popular in many areas of physics, and has even spread to other fields like biology and social sciences. We explain in the next section how the N-particle quantum system in fact converges to such a nonlinear problem in a specific limit.

3. MEAN-FIELD LIMIT TO THE GROSS–PITAEVSKII EQUATION

Gross–Pitaevskii theory. In a fully condensed system, the N bosons are by definition i.i.d. and the corresponding wave function is factorized, that is,

$$\Psi(x_1,\dots,x_N) = u^{\otimes N}(x_1,\dots,x_N) := u(x_1)\cdots u(x_N), \tag{3.1}$$

for some normalized $u \in L^2(\mathbb{R}^d,\mathbb{C})$. After some computation, one finds that the energy of such a state equals $\mathcal{E}(\Psi) = N\mathcal{E}_{\mathrm{GP}}(u)$ where $\mathcal{E}_{\mathrm{GP}}$ is the *Gross–Pitaevskii (GP) energy* [28,54],

$$\begin{aligned}\mathcal{E}_{\mathrm{GP}}(u) = &\int_{\mathbb{R}^d} \big|\nabla u(x)\big|^2\,\mathrm{d}x + \int_{\mathbb{R}^d} V(x)\big|u(x)\big|^2\,\mathrm{d}x \\ &+ \frac{\lambda(N-1)}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)\big|u(x)\big|^2\big|u(y)\big|^2\,\mathrm{d}x\,\mathrm{d}y.\end{aligned} \tag{3.2}$$

It is often also called "Hartree" when w is a smooth function. When w is proportional to a Dirac delta, one often uses the acronym NLS for "nonlinear Schrödinger." Historically designed to describe quantized vortices in superfluid helium (in which it applies to only a small fraction of the particles), the Gross–Pitaevskii model is now the main tool to study Bose–Einstein condensates. If we minimize over all normalized u, we obtain the smallest possible energy per particle of a fully condensed system

$$\boxed{e_{\mathrm{GP}} := \inf_{\int_{\mathbb{R}^d}|u|^2=1} \mathcal{E}_{\mathrm{GP}}(u).} \tag{3.3}$$

An associated minimizer u_0, when it exists, solves the nonlinear eigenvalue equation

$$\big(-\Delta + V(x) + \lambda(N-1)|u_0|^2 * w(x)\big)u_0(x) = \varepsilon_0 u_0(x), \tag{3.4}$$

where ε_0 is a Lagrange multiplier associated with the normalization constraint in $L^2(\mathbb{R}^d)$. The nonlinearity is only through the "mean-field potential" $|u_0|^2 * w$. Equation (3.4) has been used with impressive success to describe Bose–Einstein condensates. A famous example is the vortices appearing in rotating gases, see Figure 1. Note that $\mathcal{E}_{\mathrm{GP}}$ also provides a Hamiltonian system, whose dynamics is given by the nonlinear Schrödinger equation

$$i\,\partial_t u = \big(-\Delta + V + \lambda(N-1)|u|^2 * w\big)u. \tag{3.5}$$

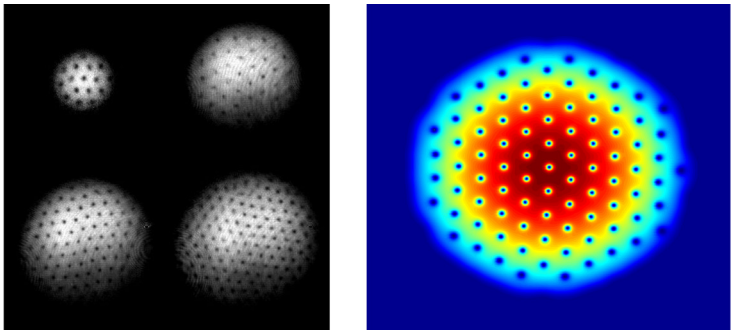

FIGURE 1
(Left) Experimental pictures of the density of fast rotating Bose–Einstein condensates from [1] (© AAAS with permission). (Right) Numerical calculation of $|u_0|^2$ for the Gross–Pitaevskii solution u_0 of (3.4) with additional terms describing the rotation, using GPELab [5] (© Antoine & Duboscq with permission). The dots are small vortices appearing under the effect of rotation, which seem to be placed on a triangular lattice [2].

Mean-field limit. The proof of Bose–Einstein condensation requires understanding how independence arises in an interacting system. The interactions will have to be weak and there are (at least) two ways this could happen. The first is when they are *rare*, which is the *dilute regime* appropriate for many experiments. Another situation is when the interactions are *small in amplitude*, that is, λ is small. In order to have them play a role, many collisions are then needed. This corresponds to a *high density regime* where the particles meet very often but interact only a little bit each time. The latter is our mean-field regime. Surprisingly, very similar theorems are expected in the two opposite regimes.

The mean-field regime corresponds to taking $N \to \infty$, with the potential V used to confine most particles to a finite region of space. At the same time, we take $\lambda \to 0$. From the formula (3.2) of the GP energy and the GP equation (3.4), we see that the interesting regime is $\lambda \sim 1/N$. This makes the quantum Hamiltonian $H_{N,\lambda}$ essentially of order N. To simplify some expressions including (3.2) and (3.4), we simply choose

$$\boxed{\lambda = \frac{1}{N-1}}$$

and denote $H_N := H_{N,\lambda}$, $E(N) = E(N,\lambda)$, etc. Then e_{GP} is independent of N. Using $E(N) \leqslant \mathcal{E}(u^{\otimes N}) = N\mathcal{E}_{\mathrm{GP}}(u)$ and minimizing over u, we obtain the simple upper bound

$$E(N) \leqslant Ne_{\mathrm{GP}}. \tag{3.6}$$

We need technical assumptions on the potentials V and w to make everything meaningful. In the whole paper we distinguish two situations:

- (*confined case*) w and $V_- = \max(0,-V)$ are in $L^p(\mathbb{R}^d,\mathbb{R}) + L^\infty(\mathbb{R}^d,\mathbb{R})$ with $p = 1$ if $d = 1$, $p > 1$ if $d = 2$ and $p = d/2$ if $d \geqslant 3$, V_+ is in $L^1_{\mathrm{loc}}(\mathbb{R}^d,\mathbb{R})$ and diverges at infinity;

- (*unconfined or locally-confined case*) V and w are in $L^p(\mathbb{R}^d,\mathbb{R})+L^\infty(\mathbb{R}^d,\mathbb{R})$ with p as above, and tend to 0 at infinity.

These conditions are not optimal and can be weakened in several ways. The most important is that we make no assumption on the sign of w or its Fourier transform $\hat{w}$. The interaction can be repulsive, attractive, or both.

Theorem 1 (Convergence of energy [37]). *Under the previous assumptions, we have*

$$\lim_{N\to\infty}\frac{E(N)}{N}=e_{\rm GP}. \tag{3.7}$$

In the confined case, if, in addition, $\int_{\mathbb{R}^d}e^{-T^{-1}V(x)}\mathrm{d}x<\infty$ *for all* $T>0$*, then we have the same limit for* $F(T,N)$ *in* (2.6)*, for all* $T>0$*.*

Similar results have been shown in many particular situations, but Theorem 1 is, to my knowledge, the first generic result. Important previous works in the same spirit include [6, 49] for unconfined systems, and [20, 55, 61] in the confined case. The limit for $F(T,N)$ says that the temperature plays no role at the considered scale. In Section 4 we look at the case where $T\to\infty$ and get a different limit. A simple proof of Theorem 1, different from that of [37], is provided in the appendix. The argument is inspired of [34, 49] and was first written in the proceedings [36] but, unfortunately, never published. It is also described in [57, CHAP. 2].

The reader should think that our model is expressed at the *macroscopic scale* where condensation happens. But interactions typically take place at the microscopic scale. After changing units, in $d=3$ the more physical dilute limit corresponds to replacing $w(x)$ by $N^3w(Nx)$ in our model. That the interaction becomes N-dependent generates many difficulties. Under further assumptions on w, the same limit (3.7) was proved in [43, 44, 46], with w replaced by $8\pi a\delta$ in $\mathcal{E}_{\rm GP}$, with $a>0$ the scattering length of w and δ the Dirac delta. The positive temperature case is handled in [16, 17].

Our next goal is to prove that the system is really condensed, that is, the bosons are essentially independent. Unfortunately, one cannot expect that Ψ_N will be close in norm to a factorized state such as (3.1). Changing one of the u's in the tensor product (that is, exciting one particle out of the condensate) would only affect the total energy to an $O(1)$ hence not change the main result. The proper way to express Bose–Einstein condensation is, following Penrose and Onsager [53], through the corresponding *k-particle density matrices*. Those are the quantum equivalent of marginals in probability theory, which appear for events involving only k particles at a time. They are defined for all $k\geqslant 1$ through their integral kernel by

$$\Gamma^{(k)}_{\Psi_N}(x_1,\dots,x_k,y_1,\dots,y_k):=\frac{N!}{(N-k)!}\int_{\mathbb{R}^{d(N-k)}}\Psi_N(x_1,\dots,x_k,Z)\overline{\Psi(y_1,\dots,y_k,Z)}\,dZ.$$

This is a compact operator with trace equal to $\frac{N!}{(N-k)!}$, hence an operator norm bounded by

$$\left\|\Gamma^{(k)}_{\Psi_N}\right\|\leqslant\frac{N!}{(N-k)!}\underset{N\to\infty}{\sim}N^k. \tag{3.8}$$

For large bosonic systems in normal conditions (such as a gas or a solid), $\Gamma^{(k)}_{\Psi_N}$ will stay of order one. Penrose and Onsager [53] suggested that a signature of Bose–Einstein condensation is when some eigenvalues are of order N^k. In fact, factorized states such as (3.1) saturate

the bound in (3.8) since their k-particle density matrices are all of rank one:

$$\Gamma^{(k)}_{u^{\otimes N}} = \frac{N!}{(N-k)!}\left|u^{\otimes k}\right\rangle\left\langle u^{\otimes k}\right|.$$

Here we use the bra-ket notation for the operator $|f\rangle\langle g|u := \langle g, u\rangle f$. The following says that, in the mean-field limit, condensation happens precisely on the set of minimizers of the Gross–Pitaevskii energy.

Theorem 2 (Convergence of states [37]). *Under the previous assumptions on V and w, let Ψ_N be any sequence such that $\langle \Psi_N, H_N \Psi_N\rangle = E(N) + o(N)$. In the* confined case*, there exist a subsequence $N_j \to \infty$ and a probability measure μ on $\mathcal{M} = \{$minimizers for $e_{\rm GP}\}$, invariant under multiplication by phase factors, such that*

$$\lim_{N_j\to\infty} \frac{\Gamma^{(k)}_{\Psi_{N_j}}}{(N_j)^k} = \int_{\mathcal{M}} \left|u^{\otimes k}\right\rangle\left\langle u^{\otimes k}\right| \mathrm{d}\mu(u), \quad \forall k \geqslant 1, \tag{3.9}$$

strongly in trace norm. In the unconfined or locally-confined case*, the result is the same except that $\mathcal{M} = \{$weak limits of minimizing sequences for $e_{\rm GP}\}$ and the limit in* (3.9) a priori *only holds weakly-$*$ in the trace class.*

The simplest case is when $\mathcal{M} = \{e^{i\theta}u_0,\ \theta \in [0, 2\pi)\}$, that is, the GP minimizer is unique modulo phase. Then there will always be complete Bose–Einstein condensation on u_0 and no need to extract subsequences. One should probably think of μ as a probability over experiments, where only one GP minimizer u_0 is usually observed at a time. Note that it is possible to construct sequences Ψ_N converging to any chosen probability μ on $\mathcal{M}$. The exact ground state of H_N might converge to a definite μ, but this is not addressed in the theorem. In the unconfined or locally-confined case, the result only gives condensation for the particles that stay in a neighborhood of the origin (due to the weak limits in the statement). All the information about the particles escaping to infinity is lost.

The main tool for proving Theorems 1 and 2 is the *quantum de Finetti theorem*. The following is our version of this result from [37], which involves weak limits and is thus stronger than the historical theorem from [33, 60].

Theorem 3 (Quantum de Finetti [33, 37, 60]). *Let Ψ_N be any sequence of normalized symmetric wave functions in $L^2_s((\mathbb{R}^d)^N, \mathbb{C})$. Assume that the k-particle density matrices satisfy*

$$\frac{\Gamma^{(k)}_{\Psi_N}}{N^k} \underset{*}{\rightharpoonup} \Upsilon^{(k)}, \quad \forall k \geqslant 1, \tag{3.10}$$

weakly-$*$ in the trace class. Then there exists a probability measure μ on the unit ball $B = \{u \in L^2(\mathbb{R}^d),\ \|u\|_{L^2} \leqslant 1\}$, invariant under multiplication by phase factors, such that

$$\Upsilon^{(k)} = \int_B \left|u^{\otimes k}\right\rangle\left\langle u^{\otimes k}\right| \mathrm{d}\mu(u), \quad \textit{for all } k \geqslant 1.$$

Convergence holds in trace norm in (3.10) *for one (hence all) $k \geqslant 1$ if and only if μ is supported on the unit sphere $S = \{u \in L^2(\mathbb{R}^d),\ \|u\|_{L^2} = 1\}$.*

The result is, in fact, valid in any separable Hilbert space, but we used $L^2(\mathbb{R}^d)$ to avoid introducing any new notation. A similar theorem appeared earlier in [3] but it was

formulated differently. Note that since the k-particle density matrices are bounded in trace norm after dividing by N^{-k}, the limit (3.10) always holds for a subsequence, by the Banach–Alaoglu theorem. Theorem 3 says that whatever converges at the scale N^k has to come from factorized states, that is, condensates. This abstract result is only a consequence of the symmetry of bosonic states and it is valid for *any* sequence Ψ_N, irrespective of the physical context. This justifies and goes much further than the theory of Penrose and Onsager [53].

The above quantum de Finetti theorem makes the proof of Theorems 1 and 2 very simple for confined systems. The main observation is that the energy can be written in terms of the two-particle density matrix as follows:

$$\frac{\mathcal{E}(\Psi_N)}{N} = \frac{\mathrm{Tr}(H_2\Gamma^{(2)}_{\Psi_N})}{2N(N-1)}.$$

After extracting a subsequence, we can assume that $N_j^{-k}\Gamma^{(k)}_{\Psi_{N_j}} \rightharpoonup_* \Upsilon^{(k)}$ weakly-$*$, for some $\Upsilon^{(k)}$ and all $k \geqslant 1$. For confined systems, H_2 has a compact resolvent and the energy bounds can be used to show that the limit holds in trace norm. Using Fatou's lemma for the trace and the quantum de Finetti Theorem 3 for $\Gamma^{(2)}$, we infer that

$$\begin{aligned}\liminf_{N\to\infty}\frac{E(N)}{N} &= \liminf_{N_j\to\infty}\frac{\mathrm{Tr}(H_2\Gamma^{(2)}_{\Psi_{N_j}})}{2N_j(N_j-1)} \geqslant \frac{1}{2}\mathrm{Tr}\big(H_2\Upsilon^{(2)}\big) = \int_S \frac{\langle u^{\otimes 2}, H_2 u^{\otimes 2}\rangle}{2}\,\mathrm{d}\mu(u)\\ &= \int_S \mathcal{E}_{\mathrm{GP}}(u)\,\mathrm{d}\mu(u) \geqslant e_{\mathrm{GP}}\int_S \mathrm{d}\mu(u) = e_{\mathrm{GP}}. \end{aligned} \tag{3.11}$$

The upper bound (3.6) implies that there is equality everywhere, hence $E(N)/N \to e_{\mathrm{GP}}$ and μ is supported on the set of minimizers for e_{GP}. This concludes the proof of Theorems 1 and 2 for confined systems. An argument of the same kind appeared before in [20, 55, 61].

For unconfined systems, some particles can escape to infinity and the argument is much more complicated. The weak limit in (3.10) might not provide sufficient information. In [37] we treated separately the particles staying in a neighborhood of 0 (for which the quantum de Finetti theorem is valid) and those that escape. All the possible cases of K particles escaping and $N-K$ staying, with K of the order of N have to be considered. These different events are handled using a technique introduced in [35] together with the concentration–compactness method. This is, in fact, also the idea of the proof of Theorem 3.

The Bogoliubov correction. The convergence of the density matrices says very little about the behavior of the wave function Ψ_N itself. This problem requires determining the next order in the energy expansion, called the Bogoliubov correction. We quickly present here the results obtained in this direction in [42]. Our idea was to concentrate on the excitations outside of the condensate. We noticed that, given a reference normalized function u_0 in $L^2(\mathbb{R}^d)$ – for instance, a GP minimizer – any N-particle wave function can be uniquely decomposed in the form

$$\Psi_N = \varphi_0 u_0^{\otimes N} + \varphi_1 \otimes_s u_0^{\otimes N-1} + \cdots + \varphi_{N-1}\otimes_s u_0 + \varphi_N \tag{3.12}$$

where the φ_j are completely orthogonal to u_0, that is, belong to $(\{u_0\}^\perp)^{\otimes j}$. Here $\otimes_s$ is a notation for the symmetrized tensor product, whose precise definition can be found in [42].

The map $\Psi_N \mapsto \varphi_0 \oplus \varphi_1 \oplus \cdots \oplus \varphi_{N-1} \oplus \varphi_N$ is a unitary operator from the N-particle space $L^2_s((\mathbb{R}^d)^N, \mathbb{C})$ to the *truncated bosonic Fock space*

$$\mathcal{F}_+^{\leqslant N} = \mathbb{C} \oplus \bigoplus_{n=1}^{N} \bigotimes_s^n \{u_0\}^\perp$$

which later became known as the *excitation map*. In the mean-field regime the φ_j's will converge to a limit in the full Fock space $\mathcal{F}_+ := \mathcal{F}_+^{\leqslant \infty}$ and describe the excitations.

We have seen that the leading order of the energy is given by the Gross–Pitaevskii minimization. Bogoliubov predicted in [9] that the next order can be expressed using the Hessian of $\mathcal{E}_{\mathrm{GP}}$ at the GP minimizer u_0, a bit like in a Taylor expansion (the gradient of $\mathcal{E}_{\mathrm{GP}}$ does not appear since u_0 is a critical point of $\mathcal{E}_{\mathrm{GP}}$ on the unit sphere). More precisely, the Hessian has to be *second-quantized* on the Fock space $\mathcal{F}_+$, which provides the so-called *Bogoliubov Hamiltonian*, defined using creation and annihilation operators by

$$\begin{aligned}\mathbb{H}_0 = &\int a^\dagger(x)\big(-\Delta + V + |u_0|^2 * w - \varepsilon_0\big)a(x)\,\mathrm{d}x \\ &+ \iint u_0(x)\overline{u_0(y)}w(x-y)a^\dagger(x)a(y)\,\mathrm{d}x\,\mathrm{d}y \\ &+ \frac{1}{2}\iint w(x-y)\big(u_0(x)u_0(y)a^\dagger(x)a^\dagger(y) + \overline{u_0(x)u_0(y)}a(x)a(y)\big)\mathrm{d}x\,\mathrm{d}y. \quad (3.13)\end{aligned}$$

It would take us too far to explain this formula in detail and we refer to [42]. The form of the spectrum of the operator $\mathbb{H}_0$ is important to explain the superfluidity of cold Bose gases. This spectrum occurs in the mean-field limit, as specified in the following result.

Theorem 4 (Validity of Bogoliubov's theory [42]). *We work in the confined case and assume that e_{GP} admits a* unique and nondegenerate *minimizer u_0 (modulo phase), which satisfies*

$$\iint_{\mathbb{R}^d\times\mathbb{R}^d} w(x-y)^2\big|u_0(x)\big|^2\big|u_0(y)\big|^2\,\mathrm{d}x\,\mathrm{d}y < \infty.$$

Then, for every fixed j, the jth eigenvalue (counted with multiplicity) satisfies

$$\lim_{N\to\infty}\big(\lambda_j(H_N) - Ne_{\mathrm{GP}}\big) = \lambda_j(\mathbb{H}_0). \quad (3.14)$$

The first eigenvalue $\lambda_1(\mathbb{H}_0)$ is always simple, with corresponding normalized ground state denoted by $\Phi = \{\varphi_n\}_{n\geqslant 0} \in \mathcal{F}_+$ (defined up to a phase factor). The lowest eigenfunction Ψ_N of H_N is also simple and, with a correct choice of phase, we have

$$\lim_{N\to\infty}\left\|\Psi_N - \sum_{n=0}^{N}\varphi_n \otimes_s (u_0)^{\otimes N-n}\right\| = 0. \quad (3.15)$$

A similar convergence holds for the higher eigenfunctions, up to subsequences in case of degeneracy.

The limit (3.15) provides the exact behavior of Ψ_N, which involves the condensate u_0 and all its excitations φ_n. That a second-quantized model arises for the excitations is well explained using the excitation map associated with the decomposition (3.12). Our result was stimulated by [25, 27, 48, 59]. Many other works followed. The similar result in the much more

complicated dilute regime has been open for a long time and was only solved very recently in several groundbreaking works [7, 8, 21, 51]. At a fixed temperature $T > 0$, Bogoliubov theory also predicts the $O(1)$ correction to Ne_{GP} in the expansion of $F(T, N, \lambda)$ in (2.6) [37].

4. DERIVATION OF NONLINEAR GIBBS MEASURES

We have seen in Theorem 2 that the condensed particles can be represented by a probability measure μ concentrated on the set $\mathcal{M}$ of minimizers of the Gross–Pitaevskii energy. This naturally raises the question of whether one can get other kinds of measures μ in a mean-field limit. Introducing a fixed temperature T as in Theorem 1 will not change anything at that scale. In [38] we proposed that taking $T \to \infty$ at a proper speed (depending on N) should lead to a *nonlinear Gibbs measure* μ and proved this in dimension $d = 1$. The much more complicated dimensions $d \in \{2, 3\}$ were only solved later in [41] and, simultaneously, in [24] with a completely different method.

Note that since we are working at the macroscopic scale, the parameter T is not the real thermodynamic temperature of the system. After reexpressing everything in microscopic units, our limit rather corresponds to looking just above the critical temperature, right before the condensation has started to appear [41, APP. B]. Thus the nonlinear Gibbs measures are describing the way that the Bose–Einstein condensate forms.

The nonlinear Gibbs measure is formally given by

$$\boxed{\mathrm{d}\mu(u) = z^{-1} e^{-\mathcal{E}_{\mathrm{GP}}(u) - \kappa \int_{\mathbb{R}^d} |u|^2} \, \mathrm{d}u,} \tag{4.1}$$

where z is a normalization factor used to make μ a probability, and where we have perturbed the GP energy by a multiple of the mass $\int_{\mathbb{R}^d} |u|^2$, for convenience. This is the same as changing V into $V + \kappa$. The constant $-\kappa$ has the physical interpretation of a chemical potential and we have $\kappa = -\varepsilon_0$ in the GP equation (3.4). From a Hamiltonian system point of view, we are considering the linear combination of two conserved quantities (energy and mass), which are both constants along the nonlinear GP flow (3.5). We could also insert a temperature in (4.1), but we have taken it equal to one to avoid introducing too many parameters.

The formula (4.1) is completely formal. There is nothing such as $\mathrm{d}u$ for functions u in infinite dimension. Things are a little bit easier if we look at the noninteracting problem, that is, take $w = 0$. In the confined case, we call $(-\Delta + V)v_j = \lambda_j v_j$ the eigenfunctions and eigenvalues of $-\Delta + V$. We then choose the constant κ so that $-\Delta + V + \kappa > 0$, that is, $\kappa > -\lambda_1(-\Delta + V)$. The formal probability measure

$$\mathrm{d}\mu_0(u) = z_0^{-1} e^{-\langle u, (-\Delta + V + \kappa)u \rangle} \, \mathrm{d}u \tag{4.2}$$

is a Gaussian measure in infinite dimension. It is by definition the unique probability measure whose cylindrical projection to the finite-dimensional space $\mathrm{span}(v_1, \dots, v_J)$ equals the normalized Gaussian on $\mathbb{C}^J$, that is,

$$\mathrm{d}\mu_{0,J}(u) := \prod_{j=1}^{J} \frac{(\lambda_j + \kappa) e^{-(\lambda_j + \kappa)|u_j|^2}}{\pi} \mathrm{d}u_j,$$

where $u_j := \langle v_j, u\rangle$, for any $J \geqslant 1$. Under appropriate growth assumptions on V, this provides a well-defined probability measure. Note, however, that we always have $\langle u, (-\Delta + V)u\rangle = +\infty$ μ_0-almost surely, which is why (4.2) is purely formal.

In dimension $d = 1$, the Gaussian measure μ_0 concentrates on functions in $L^2(\mathbb{R})$, and we can then define μ using μ_0 as reference in the form

$$\mathrm{d}\mu(u) = z^{-1} e^{-\mathcal{J}(u)}\, \mathrm{d}\mu_0(u), \tag{4.3}$$

where

$$\mathcal{J}(u) := \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \big|u(x)\big|^2 \big|u(y)\big|^2 w(x-y)\mathrm{d}x\mathrm{d}y, \quad z := \int e^{-\mathcal{J}(u)}\, \mathrm{d}\mu_0(u). \tag{4.4}$$

We will always assume that $\mathcal{J}(u) \geqslant 0$, which, for instance, follows if $w \geqslant 0$ or $\hat{w} \geqslant 0$ (defocusing case). If $\mathcal{J}(u)$ is not infinite μ_0-almost surely, we conclude that $0 < z < \infty$ and hence μ is a well-defined probability measure, absolutely continuous with respect to μ_0. The situation is much more complicated in dimensions $d \geqslant 2$, since μ_0 always concentrates on distributions. Then $|u(x)|^2$ does not make any sense and thus $\mathcal{J}(u)$ is not defined. It is necessary to remove infinities in $\mathcal{J}$ by a *renormalization procedure*.

The one-dimensional case. We first discuss the mean-field limit in dimension $d = 1$, following [38]. The Gibbs measure μ in (4.3) lives on the whole space $L^2(\mathbb{R}^d)$. It is not restricted to the unit sphere as was the case in Theorem 2. To obtain μ, we need to work grand-canonically, that is, average over all possible numbers of particles in a kind of Laplace transform. The corresponding quantum state takes the form, in Fock space,

$$\Gamma_{\kappa,\lambda,T} := Z_{\kappa,\lambda,T}^{-1} \bigoplus_{n\geqslant 0} e^{-T^{-1}(H_{n,\lambda}+\kappa n)}, \quad Z_{\kappa,\lambda,T} = 1 + \sum_{n\geqslant 1} e^{-T^{-1}\kappa n} \operatorname{Tr}(e^{-T^{-1}H_{n,\lambda}}),$$

and its density matrices are given by

$$\Gamma^{(k)}_{\kappa,\lambda,T}(X,Y) := Z_{\kappa,\lambda,T}^{-1} \sum_{n\geqslant k} \frac{n!}{(n-k)!} e^{-T^{-1}\kappa n} \int_{(\mathbb{R}^d)^{n-k}} e^{-T^{-1}H_{n,\lambda}}(X,Z;Y,Z)\, \mathrm{d}Z, \tag{4.5}$$

with $X = (x_1, \dots, x_k)$ and $Y = (y_1, \dots, y_k)$. In statistical mechanics, it is frequent to work in the grand-canonical setting, which has a much simpler algebra. It is often easy to subsequently infer a result without any average over N, but we have not yet investigated this question.

Theorem 5 (Derivation of nonlinear Gibbs measures in dimension $d = 1$ [38]). *Let $d = 1$. We work in the confined case and assume, in addition, that $\operatorname{Tr}(-\Delta + V + \kappa)^{-1} < \infty$ for some (hence all) $\kappa > -\lambda_1(-\Delta + V)$. Let $w = w_1 + w_2$ with w_1 a finite positive Borel measure on $\mathbb{R}$ and $0 \leqslant w_2 \in L^\infty(\mathbb{R})$. For any $\kappa > -\lambda_1(-\Delta + V)$ and any $k \geqslant 1$, we have the convergence*

$$\lim_{\substack{\lambda\to 0^+ \\ \lambda T \to 1}} \lambda^k \Gamma^{(k)}_{\kappa,\lambda,T} = \int \big|u^{\otimes k}\big\rangle\big\langle u^{\otimes k}\big|\, \mathrm{d}\mu(u) \tag{4.6}$$

in trace norm, where μ is the nonlinear Gibbs measure defined in (4.3).

Note the assumption that w is nonnegative, which implies $\mathcal{I}(u) \geqslant 0$. Since the number of particles has been averaged over, hence is not at our disposal anymore, the limit (4.6) involves the parameter λ with $T \sim \lambda^{-1} \to \infty$. In fact, the limit (4.6) also says that the average number of particles in the Gibbs state is of order λ^{-1}:

$$Z_{\kappa,\lambda,T}^{-1} \sum_{n\geqslant 1} n e^{-T^{-1}\kappa n} \operatorname{Tr}(e^{-T^{-1}H_{n,\lambda}}) = \operatorname{Tr}\big(\Gamma^{(1)}_{\kappa,\lambda,T}\big) \sim \lambda^{-1} \int \|u\|^2_{L^2(\mathbb{R}^d)} \mathrm{d}\mu(u).$$

The same limit as (4.6) is expected for the N-particle Gibbs state in (2.5), when $T \sim N$ and μ is replaced by its restriction to the unit sphere. The assumptions of the theorem have been weakened in [39].

Renormalization in two and three dimensions. In physics, renormalization is not just about removing undesired infinities. The removal of the bad terms must be justified by *only changing physical parameters in the system* [15, 18]. This is unfortunately often neglected in mathematical works on the subject. Here we will see that the theory can be made finite by *only adjusting the constant* κ. For simplicity, we explain the construction at the level of the GP energy, by formally manipulating infinite quantities. This will better motivate the final result in the quantum case.

Let V_0 be any potential (to be specified later) and μ_0 be the associated Gaussian measure as in (4.2) with V replaced by V_0 and $\kappa > -\lambda_1(-\Delta + V_0)$. We can renormalize the undefined $|u(x)|^2$ using *Wick ordering* [26], which formally amounts to replacing $|u(x)|^2$ by

$$:|u(x)|^2:_{\mu_0} = |u(x)|^2 - \int |u(x)|^2 \,\mathrm{d}\mu_0(u) = |u(x)|^2 - (-\Delta + V_0 + \kappa)^{-1}(x,x). \quad (4.7)$$

We hope here that the divergence of $|u(x)|^2$ is essentially independent of u, so that subtracting the average can remove it for μ_0-almost every u. Of course, the counter term is also infinite. In dimensions $d \geqslant 2$, the kernel $(-\Delta + V_0 + \kappa)^{-1}(x,y)$ of the resolvent of $-\Delta + V_0 + \kappa$, called the *Green function*, diverges when $x \to y$, at a speed depending on d. In the lower dimensions $d \in \{2,3\}$, the limit

$$\lim_{x\to y} \big((-\Delta + V_0 + \kappa)^{-1} - (-\Delta + \kappa)^{-1}\big)(x,y) \quad (4.8)$$

exists for all $\kappa > \max(0, -\lambda_1(-\Delta + V_0))$, under suitable assumptions on V_0, hence the divergence is the same as that of $(-\Delta + \kappa)^{-1}(x,y)$. Since $(-\Delta + \kappa)^{-1}$ is a translation-invariant operator, its integral kernel depends on $x - y$. It is known to diverge like $\log|x - y|^{-1}$ in dimension $d = 2$ and $|x - y|^{-1}$ in dimension $d = 3$. In dimensions $d \geqslant 4$, $(-\Delta + V_0 + \kappa)^{-1}(x,y)$ diverges like $|x - y|^{2-d}$ but there are lower divergences which remain after subtracting $(-\Delta + \kappa)^{-1}(x,y)$. With the Wick ordering (4.7), we can formally define the renormalized interaction energy by

$$\mathcal{I}_{\mathrm{r}}(u) := \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} :|u(x)|^2:_{\mu_0} :|u(y)|^2:_{\mu_0} w(x-y)\,\mathrm{d}x\,\mathrm{d}y. \quad (4.9)$$

The proper mathematical definition requires to first project u onto the finite-dimensional space spanned by the J first eigenfunctions of $-\Delta + V_0$, subtract the average against μ_0 and then take the limit $J \to \infty$, see [41]. This limit exists μ_0-almost surely in dimensions

$d \in \{2,3\}$, under suitable assumptions on V_0 and w described below. In addition, $\mathcal{J}_{\rm r}(u) \geqslant 0$ for $\hat{w} \geqslant 0$ and this allows us to define a renormalized Gibbs measure by

$$\mathrm{d}\mu_{\rm r}(u) = z_r^{-1} e^{-\mathcal{J}_{\rm r}(u)}\,\mathrm{d}\mu_0(u), \quad z_{\rm r} := \int e^{-\mathcal{J}_{\rm r}(u)}\,\mathrm{d}\mu_0(u). \tag{4.10}$$

Our initial goal was to construct and derive the (formal) measure μ in (4.1). If we just pick $V_0 = V$, then the new measure $\mu_{\rm r}$ seems very different from μ. It contains undesired additional terms in the interaction. More precisely, $\mu_{\rm r}$ involves a modified GP energy which, after expanding $\mathcal{J}_{\rm r}$, can formally be expressed as

$$\big\langle u, (-\Delta + V_0 + \kappa)u\big\rangle + \mathcal{J}_{\rm r}(u) = \big\langle u, (-\Delta + V_0 - W_{\kappa,V_0} + \kappa - \alpha)u\big\rangle + \mathcal{J}(u) + \beta, \tag{4.11}$$

where we have introduced the two infinite constants

$$\begin{aligned}
\alpha &= \int_{\mathbb{R}^d} w(x-y)(-\Delta+\kappa)^{-1}(y,y)\,\mathrm{d}y = (-\Delta+\kappa)^{-1}(0,0)\int_{\mathbb{R}^d} w = +\infty,\\
\beta &= \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} (-\Delta+V_0+\kappa)^{-1}(x,x)(-\Delta+V_0+\kappa)^{-1}(y,y)w(x-y)\mathrm{d}x\,\mathrm{d}y = +\infty,
\end{aligned} \tag{4.12}$$

as well as the finite potential

$$W_{\kappa,V_0}(x) = \int_{\mathbb{R}^d} w(x-y)\big((-\Delta+V_0+\kappa)^{-1} - (-\Delta+\kappa)^{-1}\big)(y,y)\,\mathrm{d}y.$$

The computation (4.11) suggests to search for a potential V_0 solving the nonlinear equation

$$V_0 - W_{\kappa,V_0} = V, \tag{4.13}$$

called the *counter-term problem* in [22]. Then we have the formal equality

$$\big\langle u, (-\Delta + V_0 + \kappa)u\big\rangle + \mathcal{J}_{\rm r}(u) = \mathcal{E}_{\rm GP}(u) + (\kappa - \alpha)\int_{\mathbb{R}^d} |u|^2 + \beta. \tag{4.14}$$

Adding the infinite constant β has no effect since it is then removed when we divide by z in (4.1). Our renormalized measure $\mu_{\rm r}$ thus formally coincides with the desired μ in (4.1), but with κ shifted by the infinite constant α. This shows that it is, in principle, possible to only rely on κ, if we choose a reference potential V_0 solving the nonlinear equation (4.13). A similar situation was encountered before in [29,47]. For an interpretation in terms of quasifree states, see [41]. When $\kappa \to \infty$, the nonlinear potential W_{κ,V_0} tends to 0 and the following could be proved using a Banach fixed point.

Theorem 6 (Counter-term problem [22,41]). *Let $d \in \{2,3\}$. Assume that V satisfies*

$$\frac{1+|x|^s}{C} \leqslant V(x) \leqslant C\big(1+|x|^s\big), \quad \text{for some } C > 0 \text{ and } s > \frac{2d}{d-4}, \tag{4.15}$$

and that w is an even function in $L^1(\mathbb{R}^d, (1+|x|^{2s})\,\mathrm{d}x)$ such that $\hat{w}$ is nonnegative and belongs to $L^1(\mathbb{R}^d, (1+|k|^2)\,\mathrm{d}k)$. Then there exists $\bar{\kappa}$ such that equation (4.13) admits a unique solution V_0 satisfying $V/2 \leqslant V_0 \leqslant 3V/2$, for all $\kappa > \bar{\kappa}$.

On the quantum side, there are no infinities and everything is perfectly well defined. However, we need to take a divergent sequence of constants κ in the mean-field limit, in order to account for the above renormalization of the chemical potential.

Theorem 7 (Derivation of nonlinear Gibbs measures in dimension $d \in \{2,3\}$ [24,41]). *Let $d \in \{2,3\}$ and V, w as in Theorem 6. For any $\kappa > \bar{\kappa}$, define*

$$\begin{aligned}\kappa_\lambda &:= \kappa - \frac{\int_{\mathbb{R}^d} w}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\lambda \, \mathrm{d}k}{e^{\lambda(|k|^2+\kappa)} - 1} \\ &= \begin{cases} \kappa - \frac{\log(\kappa\lambda)^{-1}}{4\pi} \int_{\mathbb{R}^d} w + o(1)_{\lambda\to 0} & \text{for } d = 2, \\ \kappa - \left(\frac{\zeta(3/2)}{8\pi^{\frac{3}{2}}\sqrt{\lambda}} - \frac{\sqrt{\kappa}}{4\pi} \right) \int_{\mathbb{R}^d} w + o(1)_{\lambda\to 0} & \text{for } d = 3. \end{cases} \end{aligned} \tag{4.16}$$

The density matrices in (4.5) satisfy

$$\lim_{\substack{\lambda\to 0^+ \\ \lambda T\to 1}} \lambda^k \Gamma^{(k)}_{\kappa_\lambda,\lambda,T} = \int \left|u^{\otimes k}\right\rangle\left\langle u^{\otimes k}\right| \mathrm{d}\mu_{\mathrm{r}}(u) \tag{4.17}$$

in Hilbert–Schmidt norm, where μ_{r} is the nonlinear Gibbs measure (4.10) with μ_0 defined using the solution V_0 of the nonlinear equation (4.13) in place of V.

The case $d = 2$ was announced earlier in [40]. We emphasize that the quantum problem in (4.5) does not contain any *ad hoc* counter term. Only the constant κ_λ is taken to $-\infty$ as in (4.16) in order to properly renormalize the interaction. The integral

$$\frac{\lambda}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{dk}{e^{\lambda(|k|^2+\kappa)} - 1} = \lambda(e^{\lambda(-\Delta+\kappa)} - 1)^{-1}(0,0)$$

appearing in (4.16) is a kind of bosonic regularization of the Green function. Note that $\lambda(e^{\lambda(-\Delta+\kappa)} - 1)^{-1} \to (-\Delta + \kappa)^{-1}$ in the sense of operators, so that we formally obtain the desired infinite shift α in (4.12) in the limit. We also remark that (4.16) is universal. It only depends on $\int_{\mathbb{R}^d} w$ and is otherwise completely independent of V and of the specific form of w. The same result holds if the $o(1)$ are dropped on the right side of (4.16).

Theorem 7 was simultaneously proved in [24], but with an approach completely different from [41]. Our proof of Theorem 7 is *variational*, like for Theorems 1 and 2. We use that the Gibbs quantum state and the measure μ are the unique minimizers of the *Gibbs variational principle*, and our goal is to prove the convergence of the quantum problem to the classical one. The link is via the quantum de Finetti Theorem 3. Passing to the limit is very delicate and requires a fine understanding of the way that singularities appear in the measure μ_{r} when $\lambda \to 0^+$. To this end, we proved new *quantum correlation inequalities* to control the localization to low momenta and reduce the problem to finite dimensions. But it would take us too far to describe this in detail here and we refer the reader to [41].

Conclusion. Bose–Einstein condensates offer a source of interesting and difficult mathematical problems. The quantum de Finetti theorem provides both a new physical interpretation of condensation and a practical mathematical tool to prove it. It also naturally led us to consider nonlinear Gibbs measures, which appear at the phase transition and describe how the condensate forms. These measures play an important role in many different mathematical and physical situations.

APPENDIX: AN ELEMENTARY PROOF OF THEOREM 1

Let us start with the case where w is continuous and has a positive Fourier transform $\hat{w} \geqslant 0$. The argument is based on the following two lemmas.

Lemma 7.1 (Hoffmann–Ostenhof inequality [32]). *For every symmetric* $\Psi_N \in H^1((\mathbb{R}^d)^N, \mathbb{C})$

$$\int_{\mathbb{R}^{dN}} |\nabla \Psi_N|^2 \geqslant N \int_{\mathbb{R}^d} |\nabla \sqrt{\rho_{\Psi_N}}|^2 \tag{4.18}$$

with the one-particle density $\rho_{\Psi_N}(x) = \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} |\Psi_N(x, x_2, \ldots, x_N)|^2 \, \mathrm{d}x_2 \cdots \mathrm{d}x_N$.

Proof. Compute $\nabla \sqrt{\rho_{\Psi_N}}$ and use the Cauchy–Schwarz inequality. ∎

Lemma 7.2 (Onsager inequality [52]). *If* $\hat{w} \geqslant 0$ *is in* $L^1(\mathbb{R}^d)$*, then, for all* $\eta \in L^1(\mathbb{R}^d)$*,*

$$\sum_{1 \leqslant j < k \leqslant N} w(x_j - x_k) \geqslant \sum_{j=1}^{N} \eta * w(x_j) - \frac{1}{2} \iint_{\mathbb{R}^{2d}} w(x-y)\eta(x)\eta(y) \, \mathrm{d}x \, \mathrm{d}y - \frac{N}{2} w(0). \tag{4.19}$$

Proof. Expand $\iint_{\mathbb{R}^{2d}} w(x-y) f(x) f(y) \, \mathrm{d}x \, \mathrm{d}y = (2\pi)^{d/2} \int_{\mathbb{R}^d} \hat{w}(k) |\hat{f}(k)|^2 \, \mathrm{d}k \geqslant 0$ with $f = \sum_{j=1}^{N} \delta_{x_j} - \eta$. ∎

With this we can prove (3.7). The potential energy can be expressed as

$$\sum_{j=1}^{N} \int_{\mathbb{R}^{dN}} V(x_j) |\Psi_N|^2 = N \int_{\mathbb{R}^d} V(x) \rho_{\Psi_N}(x) \, \mathrm{d}x.$$

Taking $\eta = N\rho_{\Psi_N}$ in (4.19) and using (4.18) provides the lower bound

$$\mathcal{E}(\Psi_N) \geqslant N \mathcal{E}_{\mathrm{GP}}(\sqrt{\rho_{\Psi_N}}) - \frac{N w(0)}{2(N-1)} \geqslant N e_{\mathrm{GP}} - \frac{N w(0)}{2(N-1)}. \tag{4.20}$$

Minimizing over Ψ_N and recalling the upper bound (3.6), we obtain

$$e_{\mathrm{GP}} - \frac{w(0)}{2(N-1)} \leqslant \frac{E(N)}{N} \leqslant e_{\mathrm{GP}}, \quad \text{for } \hat{w} \geqslant 0, \tag{4.21}$$

which clearly concludes the proof of Theorem 1, provided that $0 \leqslant \hat{w} \in L^1(\mathbb{R}^d)$. If $\hat{w}$ is nonnegative but not integrable, the proof is done by approximation.

We next turn to the case of an arbitrary w. The idea, inspired by [34, 49], is to use auxiliary classical particles repelling each other, in order to model the attractive part of the interaction. For simplicity, we consider $2N$ particles which we split in two groups of N. The positions of the N first will be denoted by $x_1, \ldots, x_N$ whereas those of the others will be denoted by $y_1 = x_{N+1}, \ldots, y_N = x_{2N}$. Of course, the separation is completely artificial and in reality the $2N$ particles are indistinguishable. We pick a $2N$-particle state Ψ_{2N} and use its bosonic symmetry in the $2N$ variables to rewrite

$$\frac{1}{2N} \int_{\mathbb{R}^{2dN}} |\nabla \Psi_{2N}|^2 = \frac{1}{N} \left\langle \Psi_{2N}, \sum_{j=1}^{N} (-\Delta)_{x_j} \Psi_{2N} \right\rangle.$$

In a similar fashion, we decompose $w = w_1 - w_2$ where $\widehat{w_1} = (\hat{w})_+ \geqslant 0$ and $\widehat{w_2} = (\hat{w})_- \geqslant 0$ and write the repulsive part using only the x_j's as

$$\frac{1}{2N(2N-1)}\left\langle \Psi_{2N}, \sum_{1\leqslant j<k\leqslant 2N} w_1(x_j - x_k)\Psi_{2N}\right\rangle$$
$$= \frac{1}{N(N-1)}\left\langle \Psi_{2N}, \sum_{1\leqslant j<k\leqslant N} w_1(x_j - x_k)\Psi_{2N}\right\rangle.$$

On the other hand, we express the attractive part as the difference of two terms, involving respectively only the y_ℓ's and both species:

$$-\frac{1}{2N(2N-1)}\left\langle \Psi_{2N}, \sum_{1\leqslant j<k\leqslant 2N} w_2(x_j - x_k)\Psi_{2N}\right\rangle$$
$$= \frac{1}{N(N-1)}\left\langle \Psi_{2N}, \sum_{1\leqslant \ell<m\leqslant N} w_2(y_\ell - y_m)\Psi_{2N}\right\rangle$$
$$-\frac{1}{N^2}\left\langle \Psi_{2N}, \sum_{j=1}^{N}\sum_{\ell=1}^{N} w_2(x_j - y_\ell)\Psi_{2N}\right\rangle.$$

This means that $\langle \Psi_{2N}, H_{2N}\Psi_{2N}\rangle/2N = \langle \Psi_{2N}, \tilde{H}_N\Psi_{2N}\rangle/N$ with

$$\tilde{H}_N = \sum_{j=1}^{N}(-\Delta)_{x_j} + V(x_j) + \frac{1}{N-1}\sum_{1\leqslant j<k\leqslant 2N} w_1(x_j - x_k)$$
$$+ \frac{1}{N-1}\sum_{1\leqslant \ell<m\leqslant N} w_2(y_\ell - y_m) - \frac{1}{N}\sum_{j=1}^{N}\sum_{\ell=1}^{N} w_2(x_j - y_\ell).$$

This Hamiltonian describes a system of N quantum particles repelling through the potential $w_1/(N-1)$ and N classical particles repelling through $w_2/(N-1)$, with an attraction $-w_2/N$ between the two species. In order to bound $\tilde{H}_N$ from below, we first fix the positions $y_1, \ldots, y_N$ of the particles in the second group and consider $\tilde{H}_N$ as an operator acting only over the x_j's. Let Φ_N be any bosonic N-particle state in the N first variables. Using (4.18) and (4.19) for the repulsive potential w_1 as in the previous proof, we obtain

$$\frac{\langle \Phi_N, \tilde{H}_N\Phi_N\rangle}{N} \geqslant \int_{\mathbb{R}^d} |\nabla\sqrt{\rho_{\Phi_N}}|^2 + V\rho_{\Psi_N} + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \rho_{\Phi_N}(x)\rho_{\Phi_N}(y)w_1(x-y)\,\mathrm{d}x\,\mathrm{d}y$$
$$- \frac{w_1(0)}{2(N-1)} + \frac{1}{N(N-1)}\sum_{1\leqslant \ell<m\leqslant N} w_2(y_\ell - y_m)$$
$$- \frac{1}{N}\sum_{\ell=1}^{N}\rho_{\Phi_N} * w_2(y_\ell).$$

Next we use again (4.19) for w_2 with $\eta = (N-1)\rho_{\Phi_N}$ and obtain

$$\sum_{1\leqslant \ell<m\leqslant N} w_2(y_\ell - y_m) - (N-1)\sum_{\ell=1}^{N}\rho_{\Phi_N} * w_2(y_\ell)$$
$$\geqslant -\frac{(N-1)^2}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \rho_{\Phi_N}(x)\rho_{\Phi_N}(y)w_2(x-y)\,dx\,dy - \frac{Nw_2(0)}{2}.$$

Therefore, we have shown that

$$\frac{\langle \Phi_N, \tilde{H}_N \Phi_N \rangle}{N} \geqslant \mathcal{E}_{\mathrm{GP}}(\sqrt{\rho_{\Phi_N}}) - \frac{w_1(0) + w_2(0)}{2(N-1)} \geqslant e_{\mathrm{GP}} - \frac{w_1(0) + w_2(0)}{2(N-1)}.$$

Since the right-hand side is independent of the y_ℓ's, we have proved the operator bound

$$\frac{\tilde{H}_N}{N} \geqslant e_{\mathrm{GP}} - \frac{w_1(0) + w_2(0)}{2(N-1)}.$$

Minimizing over Ψ_{2N} gives

$$e_{\mathrm{GP}} - \frac{w_1(0) + w_2(0)}{2(N-1)} \leqslant \frac{E(2N)}{2N} \leqslant e_{\mathrm{GP}}.$$

Note that $w_1(0) + w_2(0) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} |\hat{w}|$. We have considered an even number of particles for simplicity, but the proof works the same if we use two groups of N and $N+1$ particles. Another possibility is to use that $N \mapsto E(N)/N$ is nondecreasing, which gives, for $N \geqslant 4$,

$$\boxed{e_{\mathrm{GP}} - \frac{(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} |\hat{w}|}{N-3} \leqslant \frac{E(N)}{N} \leqslant e_{\mathrm{GP}}.} \tag{4.22}$$

Nonintegrable $\hat{w}$ can be handled using an approximation argument. ∎

Note that the two error bounds in (4.21) and (4.22) are of the optimal order $O(N^{-1})$, due to Theorem 4. If the GP minimizer exists and is unique, the convergence of the density matrices can be proved using a perturbation argument described in [57, CHAP. 2].

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