

THE INTERACTING BOSE GAS: A CONTINUING CHALLENGE

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Ever since the pioneering work of N. N. Bogoliubov in 1947, the interacting Bose gas has been a source of inspiration and a challenge to theoretical physicists striving to understand the subtleties of the quantum many-body problem. The lecture contains a survey of some mathematically rigorous results on this subject that have been obtained in the past decade. These results concern in particular the ground-state energy of a dilute Bose gas, the Gross–Pitaevskii equation for a gas in a magneto-optical trap, Bose–Einstein condensation and superfluidity, quantum phase transitions in optical lattices, and a trapped Bose gas in rapid rotation.

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INTRODUCTION

The experimental realization of Bose–Einstein condensation (BEC) in dilute, trapped alkali gases in 1995 [1, 2] has created lasting interest in the strange quantum properties exhibited by such systems. On the theoretical side the subject goes back to Einstein’s paper on BEC in ideal gases from 1924 [3], but the theory of *interacting* Bose gases began with N. N. Bogoliubov’s fundamental work of 1947 [4]. This was followed by a period of considerable activity in this field in the late 1950s and early 60s, e.g., [5]. But mathematically rigorous results were few and hard to get. In fact, after more than 60 years of theoretical investigation on interacting Bose gases, Mathematical Physics still faces the challenge to derive some of the fundamental properties of the low energy states of the many-body Hamiltonian by rigorous mathematical analysis. Substantial progress, however, has been made in the past 10 years on the following topics:

- The energy of a dilute Bose gas;
- Trapped Gases and the Gross–Pitaevskii equation;
- BEC and superfluidity in dilute, trapped gases;
- BEC and spontaneous symmetry breaking;
- Dimensional reduction in tightly confining traps;
- BEC and quantum phase transitions in optical lattices;
- Rotating gases and quantized vortices.

It is here only possible to discuss briefly a few of these topics. A general reference on the first six items from the Mathematical Physics point of view is [6], while the monograph [7] is devoted to rotating gases. See also [8–11] for some recent results on rotating gases and further references.

1. THE MATHEMATICAL SETTING

The basic quantum mechanical Hamiltonian for N particles in \mathbb{R}^3 that interact via a pair potential v and are trapped in an external potential V is

$$H = \sum_{j=1}^N (-\nabla_j^2 + V(\mathbf{x}_j)) + \sum_{1 \leq i < j \leq N} v(\mathbf{x}_i - \mathbf{x}_j). \tag{1}$$

Here $\mathbf{x}_i \in \mathbb{R}^3, i = 1, \dots, N$ are the positions of the particles and units are chosen so that $\hbar = 2m = 1$. We shall always assume that $v = v(|\mathbf{x}|)$ is *nonnegative* and of finite range (or, more generally, decreases faster than $|x|^{-3}$ at infinity). Moreover, the confining potential V is assumed to be continuous with $V(\mathbf{x}) \rightarrow \infty$ for $|\mathbf{x}| \rightarrow \infty$. When studying superfluidity and rotating systems the Laplacian $-\nabla_j^2$ is replaced by a magnetic Laplacian $(i\nabla_j + \mathbf{A}(\mathbf{x}_j))^2$, where \mathbf{A} is a vector potential.

We focus on *spinless bosons* where the Hamiltonian operates on symmetric wave functions in $L^2(\mathbb{R}^{3N}, d\mathbf{x}_1 \cdots d\mathbf{x}_N)$. For ultracold gases the normalized ground-state wave function $\Psi_0(\mathbf{x}_1, \dots, \mathbf{x}_N)$ of H and the corresponding reduced one-particle density matrix

$$\rho_0^{(1)}(\mathbf{x}, \mathbf{x}') = N \int_{\mathbb{R}^{3(N-1)}} \Psi_0(\mathbf{x}, \mathbf{x}_2, \dots, \mathbf{x}_N) \Psi_0^*(\mathbf{x}', \mathbf{x}_2, \dots, \mathbf{x}_N) d\mathbf{x}_2 \cdots d\mathbf{x}_N \tag{2}$$

are of particular interest. *Bose–Einstein condensation* in the ground state means, by definition, that the operator defined by the integral kernel $\rho_0^{(1)}(\mathbf{x}, \mathbf{x}')$ has an eigenvalue of the order N for all large N . It is important to remark that the definition of BEC is only precise if the N dependence of the parameters involved has been specified. Important cases are:

- **Thermodynamic limit:** The particles are confined in a box Λ with volume $|\Lambda| \rightarrow \infty$ as $N \rightarrow \infty$ with constant density $\rho = N/|\Lambda|$.
- **Gross–Pitaevskii limit:** $N \rightarrow \infty, Na/L = \text{const}$, with a the *scattering length* of v (see below) and L the length scale associated with $-\nabla^2 + V$. Special case: box Λ and $L = |\Lambda|^{1/3}$. Note: $Na/L = a\rho/(L^{-2})$.
- **«Thomas–Fermi» limit:** $N \rightarrow \infty, Na/L \rightarrow \infty$, but $Na^3/L^3 \rightarrow 0$.

2. THE GROUND-STATE ENERGY

Consider a spherically symmetric pair interaction potential v of short range. The *scattering length* of v , denoted by a , is defined by considering the zero energy scattering equation

$$-\nabla^2\psi + \frac{1}{2}v\psi = 0.$$

For $r = |\mathbf{x}|$ larger than the range of v , the solution has the form $\psi(r) = (\text{const})(1 - (a/r))$. In particular, if the constant is chosen to be 1, partial integration, and $v \geq 0$, gives

$$8\pi a = \int \{2|\nabla\psi|^2 + |\psi|^2v\} \leq \int v. \quad (3)$$

If $v \geq 0$ the scattering length determines completely the ground-state energy $E^{\text{QM}}(2, L)$ of a pair of bosons in a large box Λ of side length $L \gg a$, namely $E^{\text{QM}}(2, \Lambda) \approx 8\pi a/L^3$. Consider now for $v \geq 0$ the Hamiltonian of N bosons in a box Λ of side length L with appropriate boundary conditions:

$$H = -\sum_{j=1}^N \nabla_j^2 + \sum_{1 \leq i < j \leq N} v(\mathbf{x}_i - \mathbf{x}_j). \quad (4)$$

Denoting its ground-state energy by $E^{\text{QM}}(N, L)$, the energy per particle in the thermodynamic limit with $\rho = N/L^3$ fixed is $e_0(\rho) = \lim_{N \rightarrow \infty} E^{\text{QM}}(N, L)/N$. In dilute gases the *low density asymptotics* of $e_0(\rho)$ is of importance, where *low density* means that $\rho a^3 \ll 1$; i.e., the scattering length a is much smaller than the mean particle distance, $\rho^{-1/3}$. The basic formula for the ground-state energy of a dilute Bose gas is [12]

Theorem 1 (Ground-state energy). For $a^3\rho \ll 1$

$$e_0(\rho) = 4\pi a\rho(1 + o(1)). \quad (5)$$

Heuristically, the formula (5) can be motivated by arguing that in dilute gases all particle pairs should be treated as approximately independent which leads to $E^{\text{QM}}(N, L) \approx (1/2)N(N-1)E^{\text{QM}}(2, L) \approx (1/2)N^2 8\pi a/L^3 = N 4\pi a\rho$. This heuristic argument is, however, very far from a rigorous proof because the ground state is in general highly correlated. In fact, the analogous heuristic reasoning in two dimensions gives the *wrong* answer [13, 14]. The formula (5) has an interesting history and it took almost 70 years to establish it rigorously. It first appeared in [15] (for a gas of hard balls) and Bogoliubov's fundamental paper [4] contains a version of it with $8\pi a$ replaced by the right-hand side of (3), i.e., the first-order perturbative approximation. A rigorous upper bound was given by

Dyson in 1957 [16], but an asymptotically correct lower bound was not obtained until 40 years later [12]. Recently, there has been renewed interest in higher order corrections to (5) that were computed with various approximation techniques in the 50s and 60s [5], and some rigorous estimates going beyond (5) have been obtained in [17] and [18].

The basic reason why it is so difficult to bound the energy from below is that the energy is very small if the density is low. Also, one should bear in mind that there are really two physically different regimes to consider:

1. «Hard potential», i.e., v large (in particular hard core). The energy is here *mostly kinetic* (due to the bending of the wave function when two particles come close to each other) and ground state is *highly correlated*. In this regime perturbation theory does not apply.

2. «Soft potential», i.e., v small. The energy is here *mostly potential* because the wave function is approximately constant. Lowest-order perturbation theory (with the *uncorrelated*, unperturbed state $\Psi_0 = L^{-3N/2}$) gives $e_0(\rho) \approx (1/2)\rho \int v(\mathbf{x}) d^3\mathbf{x}$. This cannot be the right answer (it is independent of \hbar and m !), but it is at least the first Born approximation to $4\pi a\rho$. (Note that a depends on \hbar and m .) It is *a priori* not at all obvious that the same formula, Eq. (5), applies both to «hard» and to «soft» potentials.

In [16] Dyson succeeded in transforming Regime 1 into Regime 2 (for hard spheres) by sacrificing the kinetic energy. In this way he obtained a lower bound $\sim \rho a$, but the factor in front was only about 1/14 of the optimal one. His idea of replacing a hard potential by a soft one was, however, taken up in [12] and led, in combination with other ingredients, eventually to an asymptotically correct lower bound. Dyson's idea has, in fact, been a key element in many of the subsequent developments, in particular the proof of BEC and superfluidity in the GP limit in [19] and [20] respectively, and the dimensional reduction of a gas in a tightly confining trap [21, 22].

3. GROSS-PITAEVSKII THEORY

Consider now the N -body Hamiltonian (20) with an external potential V , representing a confining trap. This potential comes with a natural length scale $L = e_V^{-1/2}$, where e_V is the spectral gap of $-\nabla^2 + V$. It is natural to study the ground-state properties of H , and in particular BEC, in the *Gross-Pitaevskii (GP) limit* where $N \rightarrow \infty$ with a *fixed* value of the *GP interaction parameter*

$$g \equiv \frac{4\pi Na}{L} \approx \frac{e_0(\rho)}{e_V} \tag{6}$$

with $\rho = N/L^3$. Note that $a^3\rho \sim g/N^2 = O(1/N^2)$ if g is fixed, so the GP limit is a special case of a dilute limit, with the interaction energy of the same order as the spectral gap of the Hamiltonian without interaction.

The GP limit can be achieved either by keeping a fixed and scaling the external potential V so that $L \sim N$, or by keeping V fixed and taking $a \sim N^{-1}$. The latter can formally be regarded as a scaling of the interaction potential, i.e., writing $v(r) = N^2 v_1(Nr)$ with v_1 fixed. Note that this is the *opposite of the usual mean field limit* where the potential is scaled with N as $v(r) = N^{-3} v_1(r/N)$. In fact, the technique for deriving the GP equation below from the many-body Hamiltonian is quite different from mean field techniques.

In the GP limit the ground state can be described by minimizing a functional of functions on \mathbb{R}^3 , the *GP energy functional*

$$\mathcal{E}^{\text{GP}}[\varphi] = \int_{\mathbb{R}^3} (|\nabla\varphi|^2 + V|\varphi|^2 + g|\varphi|^4) \quad (7)$$

with the subsidiary condition $\int |\varphi|^2 = 1$. A motivation for the term $g|\varphi|^4$ comes from (5): With $\rho(\mathbf{x}) = N|\varphi(\mathbf{x})|^2$ the local density, we have $Ng \int |\varphi|^4 = 4\pi a \int \rho(\mathbf{x})^2$, and $4\pi a \rho(\mathbf{x})^2$ is the interaction energy per unit volume.

The minimizer, denoted φ^{GP} , of the GP functional is the unique, nonnegative solution of the (time-independent) *Gross–Pitaevskii equation*

$$(-\nabla^2 + V + 2g|\varphi|^2)\varphi = \mu\varphi \quad (8)$$

with a Lagrange multiplier (chemical potential) μ . The energy corresponding to φ^{GP} is

$$E_g^{\text{GP}} = \mathcal{E}^{\text{GP}}[\varphi^{\text{GP}}] = \inf \left\{ \mathcal{E}^{\text{GP}}[\varphi] : \int |\varphi|^2 = 1 \right\}. \quad (9)$$

Basic results in GP theory are the following theorems [19, 24]:

Theorem 2 (GP energy asymptotics). *If $N \rightarrow \infty$ with g fixed (i.e., $a \sim N^{-1}L$), then*

$$\frac{E^{\text{QM}}(N, a)}{NE_g^{\text{GP}}} \rightarrow 1. \quad (10)$$

Theorem 3 (BEC in the GP limit). *If $N \rightarrow \infty$ with g fixed, then*

$$\frac{1}{N}\rho_0^{(1)}(\mathbf{x}, \mathbf{x}') \rightarrow \varphi^{\text{GP}}(\mathbf{x})\varphi^{\text{GP}}(\mathbf{x}'), \quad (11)$$

where the convergence is in trace norm.

In other words: There is *complete BEC in the GP limit* and φ^{GP} is the wave function of the condensate. As a corollary one sees that in the GP limit the normalized particle density of the many-body ground state converges to $N|\varphi^{\text{GP}}(\mathbf{x})|^2$ and the momentum density to $N|\tilde{\varphi}^{\text{GP}}(\mathbf{p})|^2$, where $\tilde{\varphi}^{\text{GP}}$ denotes the Fourier transform of φ^{GP} .

We present here a very brief sketch of the proof of BEC in the GP limit [19] for the special case when the trap is a box Λ of side length L : With Ψ_0 the many-body ground-state wave function, we employ the notation $\mathbf{X} = (\mathbf{x}_2, \dots, \mathbf{x}_N)$, $\psi_{\mathbf{X}}(\mathbf{x}) = \Psi_0(\mathbf{x}, \mathbf{X})$. Moreover, we denote by N_0 the average occupancy of the constant single particle ground state of the Laplacian in Λ . In terms of the one-particle density matrix (2) the *depletion of the condensate* can be written as

$$1 - \frac{N_0}{N} = 1 - (NL^3)^{-1} \int \int \rho^{(1)}(\mathbf{x}, \mathbf{x}') d\mathbf{x} d\mathbf{x}' = \int d\mathbf{X} \|\psi_{\mathbf{X}} - \langle \psi_{\mathbf{X}} \rangle\|_{L^2(\Lambda)}^2, \quad (12)$$

where $\langle f \rangle = L^{-3} \int_{\Lambda} f$. The proof that the depletion tends to zero in the GP limit has two main ingredients. One is a generalization of the simple *Poincaré inequality* [25]

$$\|f - \langle f \rangle\|_{L^2(\Lambda)}^2 \leq CL^2 \|\nabla f\|_{L^2(\Lambda)}^2, \quad (13)$$

namely the following inequality if $\Omega \subset \Lambda$:

$$\|f - \langle f \rangle\|_{L^2(\Lambda)}^2 \leq C_1 L^2 \|\nabla f\|_{L^2(\Omega)}^2 + C_2 |\Omega^c|^{2/3} \|\nabla f\|_{L^2(\Lambda)}^2. \quad (14)$$

Equation (14) is easily obtained from the Poincaré–Sobolev inequality ([25], Thm. 8.12)

$$\|f - \langle f \rangle\|_{L^2(\Lambda)}^2 \leq C \|\nabla f\|_{L^{6/5}(\Lambda)}^2, \quad (15)$$

in combination with Hölder’s inequality.

The other ingredient in the proof of BEC is *localization of the kinetic energy*: While

$$\int d\mathbf{X} \|\nabla \psi_{\mathbf{X}}\|^2 \sim \rho a(1 + o(1)), \quad (16)$$

it can be shown that there is an $\Omega \subset \Lambda$ such that $|\Omega^c|/L^3 = o(1)$ and

$$(\rho a)^{-1} \int d\mathbf{X} \|\nabla \psi_{\mathbf{X}}\|_{L^2(\Omega)}^2 = o(1). \quad (17)$$

This is a highly nontrivial result but it can be extracted from the proof of the ground-state energy in [12]. Given Eqs. (12), (14) and (17), the proof of BEC follows:

$$1 - \frac{N_0}{N} \leq L^2 \rho a \times o(1) = \frac{Na}{L} \times o(1) \rightarrow 0, \quad (18)$$

if $N \rightarrow \infty$ with $g = Na/L$ fixed. It should be noted that the depletion (18) may tend to zero even if the GP parameter tends to ∞ as $N \rightarrow \infty$, but only if the increase of the latter is compensated by the factor $o(1)$ that tends to zero with ρa^3 . The estimates on this factor in [12] are rather crude and one is still far from proving BEC in the full «Thomas–Fermi» limit mentioned in Sec. 1, let alone in the *thermodynamic limit* where complete BEC is not expected. Proving

BEC in the thermodynamic limit is, in fact, still one of the outstanding challenges in the theory of interacting Bose gases. Its difficulty can partly be understood from the fact that BEC is always accompanied by the breaking of a continuous gauge symmetry [23] and phase transitions are notoriously difficult to derive in the presence of continuous symmetries.

4. ROTATING GASES AND VORTICES

Consider now a gas in a container that rotates with angular velocity Ω . The Hamiltonian in the rotating frame is

$$H = \sum_{j=1}^N \left(-\nabla_j^2 + V(\mathbf{x}_j) - \mathbf{L}_j \cdot \Omega \right) + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|), \quad (19)$$

where $\mathbf{L}_j = -i\mathbf{x}_j \wedge \nabla_j$ is the angular momentum operator of particle j . The Hamiltonian can alternatively be written in the form

$$H = \sum_{j=1}^N \left((i\nabla_j + \mathbf{A}(\mathbf{x}_j))^2 + V(\mathbf{x}_j) - \frac{1}{4}\Omega^2 r_j^2 \right) + \sum_{1 \leq i < j \leq N} v(|\mathbf{x}_i - \mathbf{x}_j|), \quad (20)$$

with $\mathbf{A}(\mathbf{x}) = \frac{1}{2}\Omega \wedge \mathbf{x}$ and r = distance from the rotation axis. The corresponding Gross–Pitaevskii energy functional in the rotating case is

$$\mathcal{E}^{\text{GP}}[\varphi] = \int_{\mathbb{R}^3} \left\{ |(i\nabla + \mathbf{A})\varphi|^2 + \left(V - \frac{1}{4}\Omega^2 r \right) |\varphi|^2 + g|\varphi|^4 \right\}. \quad (21)$$

The GP energy $E_{g,\Omega}^{\text{GP}}$, i.e., the infimum of (21) for normalized wave functions, now depends on the rotation velocity Ω besides the GP parameter g . A new phenomenon compared to the nonrotating case is that the minimizer may have a nontrivial phase and it need not be unique. The basic results on the relation between the Hamiltonian (19) and GP theory were obtained in [26] and [27]:

Theorem 4 (Energy asymptotics in GP limit, Ω fixed). *If $N \rightarrow \infty$ with g and Ω fixed, then*

$$\frac{E^{\text{QM}}(N, a, \Omega)}{NE_{g,\Omega}^{\text{GP}}} \rightarrow 1. \quad (22)$$

Theorem 5 (BEC in GP limit, Ω fixed). *If $N \rightarrow \infty$ with g and Ω fixed, then the convex hull of the projectors onto GP minimizers coincides with the possible $N \rightarrow \infty$ limits of one-particle density matrices of N -particle ground states.*

The technique of the proof of these theorems is by necessity rather different from the one originally used in the nonrotating case [24], the reason being that the many-body wave functions are no longer real valued (in general), and the phase factor prevents localization of the particles. The leading order asymptotics in the «Thomas–Fermi» limit, where $g \rightarrow \infty$ (and possibly also $\Omega \rightarrow \infty$), was studied in [28].

The GP minimizers are solutions of the GP equation for rotating gases

$$\left\{ -(\nabla + i\mathbf{A})^2 + \left(V - \frac{1}{4}\Omega^2 r^2 \right) + 2g|\varphi|^2 \right\} \varphi = \mu\varphi. \quad (23)$$

An important new feature compared to the nonrotating case is the possible occurrence of *vortices*, i.e., singularities of the phase of φ with integer winding numbers. The vortices may be associated with spontaneous breaking of rotational symmetry of the trap. The GP equation and its vortex solutions is a subject of its own that can be studied independently of the many-body problem. The most detailed results are for the 2D equation and $g \rightarrow \infty$ [7]. We refer to [10, 29, 30] for some recent results where g and Ω both tend to ∞ in *anharmonic* traps, i.e., for V increasing more rapidly than quadratically with the distance from the rotation axis.

A very interesting situation occurs for a *quadratic* trap potential, $V(\mathbf{x}) = (1/2)\Omega_{\text{osc}}^2 |\mathbf{x}|^2$, when Ω approaches the *critical frequency*

$$\Omega_c = \sqrt{2}\Omega_{\text{osc}}, \quad (24)$$

at which $V(\mathbf{x}) - (1/4)\Omega^2 r^2$ is no longer bounded below. It is convenient to choose units so that $\Omega_c = 1$. As $\Omega \rightarrow 1$, the system becomes effectively two-dimensional with an effective radius R tending to infinity. In fact, equating the potential energy $\sim (1 - \Omega)^2 R^2$ and the interaction energy per particle $\sim NaR^{-2}$ gives the estimate

$$R^2 \sim \left(\frac{Na}{1 - \Omega} \right)^{1/2}. \quad (25)$$

Interpreting Ω as a vortex density (that is, strictly speaking, only justified when there is a large number of vortices), one may define a *filling factor* as

$$\nu = \frac{\# \text{ particles}}{\# \text{ vortices}} \sim \frac{N}{\Omega R^2} \sim \left(\frac{N(1 - \Omega)}{a} \right)^{1/2}. \quad (26)$$

The expectations are [8, 9]:

- If $\nu \rightarrow \infty$, there is a GP description with a GP equation restricted to wave functions in the *lowest Landau Level* (LLL) of the magnetic Laplacian.
- If ν stays small, the many-body ground state is highly correlated and there is *no GP description*. Instead, the wave functions should be bosonic analogues of

the fermionic wave functions that occur in the theory of the Fractional Quantum Hall Effect in the LLL.

In particular, at filling factor $1/2$ the wave function should be well approximated by a *Laughlin type* function

$$\Psi \sim \prod_{i<j}^N (z_i - z_j)^2 \prod_{i=1}^N \exp(-|z_i|^2/4), \quad (27)$$

where $z_j = x_j + iy_j \in \mathbb{C}$ denote the particle positions in $\mathbb{R}^2 \simeq \mathbb{C}$.

For filling factors between $1/2$ and ∞ , rich physics is expected. A model for studying these phenomena is a many-body Hamiltonian restricted to the LLL:

$$H_{\text{LLL}} = (1 - \Omega) \sum_{i=1}^N z_i \frac{\partial}{\partial z_i} + 4\pi a \sum_{i<j} \delta_{ij}, \quad (28)$$

operating on the Bargmann space of analytic functions that are square integrable w.r.t. the measure $\exp(-\sum_i |z_i|^2) d^2 z_1 \cdots d^2 z_N$, and where δ_{ij} denotes the projection of $\delta(z_i - z_j)$ on this space. This model has recently been rigorously derived from the full 3D many-body Hamiltonian [31], and its limit for $\nu \rightarrow \infty$, corresponding to $a/(N(1 - \Omega)) \rightarrow 0$, has been analyzed in [32], leading to a GP equation for wave functions in the LLL. The properties of the solutions of this GP equation have been studied in many papers, including [33], where further references can be found.

CONCLUSIONS

In this contribution some results on a few of the topics mentioned in the Introduction have been reviewed. While these results are only a tiny fraction of the extensive theoretical work on cold quantum gases that has been carried out since 1995, they demonstrate the possibility to extract physically relevant properties of the many-body Hamiltonian (20) by rigorous mathematical analysis. Such an endeavor is very much in the spirit of N.N. Bogoliubov's pioneering work [4], but it should be noted that a rigorous justification of the pairing theory that lies behind his approximation has so far only been obtained in the special case of the charged Bose gas at high density [34,35]. A better understanding of this aspect for dilute gases with short-range interactions might be an essential step towards a solution of *the* outstanding open problem in the theory of cold gases: to prove BEC in the thermodynamic limit for a continuous model with realistic interactions.

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