The Ground State Energy and Density of Interacting Bosons in a Trap

Elliott H. Lieb[1], Robert Seiringer[2] and Jakob Yngvason[2]

[1]Departments of Physics and Mathematics, Princeton University,
P. O. Box 708, Princeton, New Jersey 08544-0708, USA
[2] Institut für Theoretische Physik, Universtität Wien,
Boltzmanngasse 5, A-1090 Wien, Austria

Abstract

In the theoretical description of recent experiments with dilute Bose gases confined in external potentials the Gross-Pitaevskii equation plays an important role. Its status as an approximation for the quantum mechanical many-body ground state problem has recently been rigorously clarified. A summary of this work is presented here.

1 Introduction

The Gross-Pitaevskii (GP) equation is a nonlinear Schrödinger equation that was introduced in the early sixties [1]–[3] as a phenomenological equation for the order parameter in superfluid He_4. It has come into prominence again because of recent experiments on Bose-Einstein condensation of dilute gases in magnetic traps. The paper [4] brings an up to date review of these developments.

One of the inputs needed for the justification of the GP equation starting from the many body Hamiltonian is the ground state energy of a a dilute, thermodynamically infinite, homogeneous Bose gas. The formula for this quantity is older than the GP equation but it has only very recently been derived rigorously for suitable interparticle potentials. See [5] and [6]. The paper [7] goes one step further and derives the GP as a limit of the full quantum mechanical description. This derivation is summarized in the present contribution.

The starting point of the investigation is the Hamiltonian for N bosons that interact with each other via a spherically symmetric pair-potential $v(|\vec{x}_i - \vec{x}_j|)$ and are confined by an external potential $V(\vec{x})$:

$$H = \sum_{i=1}^{N} \{-\Delta_i + V(\vec{x}_i)\} + \sum_{1\leq i<j\leq N} v(|\vec{x}_i - \vec{x}_j|). \tag{1.1}$$

The Hamiltonian acts on *symmetric* wave functions in $L^2(\mathbf{R}^{3N}, d^{3N}x)$. The pair interaction v is assumed to be *nonnegative* and of short range, more precisely, $v(r) \leq (\text{const.})\, r^{-(3+\varepsilon)}$ as $r \to \infty$, for some $\varepsilon > 0$. The potential V that represents the trap is continuous and $V(\vec{x}) \to \infty$ as $|\vec{x}| \to \infty$. By shifting the energy scale we can assume that $\min_{\vec{x}} V(\vec{x}) = 0$.

Units are chosen so that $\hbar = 2m = 1$, where m is the particle mass. A natural energy unit is given by the ground state energy $\hbar\omega$ of the one particle Hamiltonian $-(\hbar^2/2m)\Delta + V$. The corresponding length unit, $\sqrt{\hbar/(m\omega)}$, measures the effective extension of the trap.

The ground state wave function $\Psi_0(\vec{x}_1, \ldots, \vec{x}_N)$ satisfies $H\Psi_0 = E^{\rm QM}\Psi_0$, with the ground state energy $E^{\rm QM} = \inf \operatorname{spec} H$. If $v = 0$, then $\Psi_0(\vec{x}_1, \ldots, \vec{x}_N) = \prod_{i=1}^{N} \Phi_0(\vec{x}_i)$, with Φ_0 the ground state wave function of $-\Delta + V(\vec{x})$. On the other hand, if $v \neq 0$ the ground state $\Psi_0(\vec{x}_1, \ldots, \vec{x}_N)$ is, in general, far from being a product state if N is large. In spite of this fact, recent experiments on BE condensation are usually interpreted in terms of a function $\Phi^{\rm GP}(\vec{x})$ of a single $\vec{x} \in \mathbb{R}^3$, the solution of the *Gross-Pitaevskii equation*

$$(-\Delta + V + 8\pi a|\Phi|^2)\Phi = \lambda\Phi, \tag{1.2}$$

together with the normalization condition

$$\int_{\mathbb{R}^3} |\Phi(\vec{x})|^2 = N. \tag{1.3}$$

Here a is the *scattering length* of the potential v:

$$a = \lim_{r\to\infty} \left(r - \frac{u_0(r)}{u_0'(r)} \right) \tag{1.4}$$

where u_0 satisfies the zero energy scattering equation,

$$-u''(r) + \tfrac{1}{2} v(r) u(r) = 0, \tag{1.5}$$

and $u_0(0) = 0$. (The factor $1/2$ is due to the reduced mass of the two-body problem.) The GP equation (1.2) is the variational equation for the minimization of the GP *energy functional*

$$\mathcal{E}^{\rm GP}[\Phi] = \int \left(|\nabla\Phi|^2 + V|\Phi|^2 + 4\pi a|\Phi|^4\right) d^3\vec{x} \tag{1.6}$$

with the subsidiary condition (1.3). The corresponding energy is

$$E^{\rm GP}(N,a) = \inf_{\int|\Phi|^2=N} \mathcal{E}^{\rm GP}[\Phi] = \mathcal{E}^{\rm GP}[\Phi^{\rm GP}], \tag{1.7}$$

with a unique, positive $\Phi^{\rm GP}$. The eigenvalue, λ, in (1.2) is related to $E^{\rm GP}$ by

$$\lambda = dE^{\rm GP}(N,a)/dN = E^{\rm GP}(N,a)/N + 4\pi a\bar{\rho}, \tag{1.8}$$

where

$$\bar{\rho} = \frac{1}{N}\int |\Phi^{\rm GP}(\vec{x})|^4 d^3\vec{x} \tag{1.9}$$

is the *mean density.* The minimizer $\Phi^{\rm GP}$ of (1.6) with the condition (1.3) depends on N and a, of course, and when this is important we denote it by $\Phi^{\rm GP}_{N,a}$.

Mathematically, the GP equation is quite similar to the Thomas-Fermi-von Weizsäcker equation [8] and its basic properties can be established by similar means. See [7], Sect. 2 and Appendix A.

The idea is now that for *dilute* gases one should have

$$E^{\rm GP} \approx E^{\rm QM} \quad \text{and} \quad \rho^{\rm QM}(\vec{x}) \approx \left|\Phi^{\rm GP}(\vec{x})\right|^2 \equiv \rho^{\rm GP}(\vec{x}), \tag{1.10}$$

where the quantum mechanical particle density in the ground state is defined by

$$\rho^{\rm QM}(\vec{x}) = N\int |\Psi_0(\vec{x},\vec{x}_2,\dots,\vec{x}_N)|^2 d\vec{x}_2\cdots d\vec{x}_N. \tag{1.11}$$

Dilute means here that

$$\bar{\rho}a^3 \ll 1. \tag{1.12}$$

The task is to make (1.10) precise and prove it!

The first remark is that by scaling

$$E^{\rm GP}(N,a) = NE^{\rm GP}(1,Na) \quad \text{and} \quad \Phi^{\rm GP}_{N,a} = N^{1/2}\Phi^{\rm GP}_{1,Na}. \tag{1.13}$$

Hence Na is the natural parameter in GP theory. It should also be noted that $E^{\rm QM}$ depends on N and v and not only on the scattering length a. However, in the limit we are about to define, it is really only a that matters. To bring this out we write

$$v(r) = (a_1/a)^2 v_1(a_1 r/a), \tag{1.14}$$

where v_1 has scattering length a_1 and regard v_1 as *fixed.* Then $E^{\rm QM}$ is a function $E^{\rm QM}(N,a)$ of N and a and we can state our main result.

Theorem 1.1 (Dilute limit of the QM ground state energy and density).

$$\lim_{N\to\infty} \frac{E^{\rm QM}(N,a)}{E^{\rm GP}(N,a)} = 1 \tag{1.15}$$

and

$$\lim_{N\to\infty} \frac{1}{N}\rho^{\rm QM}_{N,a}(\vec{x}) = \left|\Phi^{\rm GP}_{1,Na}(\vec{x})\right|^2 \tag{1.16}$$

if Na is fixed. The convergence in (1.16) is in the weak L_1-sense.

In particular, the limits depend only on the scattering length $a_1 = Na$ of v_1 and not on details of the potential.

Remark. Since $\bar\rho \sim N$ the attribute 'dilute' may seem a bit strange for these limits. However, what matters is that the scattering length a is small compared to the mean particle distance, $\sim \bar\rho^{1/3}$, and if Na is kept constant, then $\bar\rho a^3 \sim N^{-2}$. It is also important to remember that the unit of length, $\sqrt{\hbar/(m\omega)} \equiv a_{\rm trap}$, depends on the external potential, and a really stands for $a/a_{\rm trap}$. If the external potential is scaled with N, the both $a_{\rm trap}$ and the energy unit $\hbar\omega$ depend on N. For instance, in order to achieve a finite transition temperature for the BE condensation of a noninteracting gas in a parabolic trap it is necessary to keep $N\omega^3$ fixed in the thermodynamic limit, and hence $a_{\rm trap} \sim N^{1/6}$ and $\hbar\omega \sim N^{-1/3}$. (See [4], Eq. (14).) However, since the energy unit cancels in (1.15) a dependence of V on N does not affect the validity of (1.15), and (1.16) also remains valid taking into account that both sides really contain the factor $a_{\rm trap}^{-3}$.

2 The dilute homogeneous Bose gas

The motivation for the last term in the GP energy functional (1.6) is an asymptotic formula for the quantum mechanical ground state energy $E_0(N,L)$ of N bosons in a rectangular *box* of side length L (i.e., the *homogeneous* case), that was put forward by several authors many decades ago. Consider the energy per particle in the thermodynamic limit with $\rho = N/L^3$ fixed:

$$e_0(\rho) = \lim_{L\to\infty} E_0(\rho L^3, L)/(\rho L^3). \tag{2.1}$$

According to the pioneering work of Bogoliubov [9] the leading term in the *low density asymptotics* of $e_0(\rho)$ is given by

$$e_0(\rho) \approx 4\pi\rho a \tag{2.2}$$

for $\rho a^3 \ll 1$. In the 50's and early 60's several derivations of this formula were presented [10].They all depended on some special assumptions about the ground state that have never been proved or the selection of some special terms from a perturbation expansion that most likely diverges. The only rigorous estimates of this period were obtained by Dyson [11] for hard spheres:

$$\frac{1+2Y^{1/3}}{(1-Y^{1/3})^2} \geq \frac{e_0(\rho)}{4\pi\rho a} \geq \frac{1}{10\sqrt{2}} \tag{2.3}$$

with $Y \equiv 4\pi\rho a^3/3$. The upper bound has the right asymptotic form, and it is not very difficult to generalize it to other potentials than hard spheres. The lower bound on the other hand is too low by a factor of about 1/14 and a remedy for this situation was obtained only 40 years after Dyson's paper:

Theorem 2.1 (Lower bound for a homogeneous gas). *If v is nonnegative and of finite range, then*

$$\frac{e_0(\rho)}{4\pi\rho a} \geq (1 - C\,Y^{1/17}) \tag{2.4}$$

with some constant C.

The proof of this theorem is given in [5], see also the exposition in [6]. For the application to the proof of Theorem 1.1 we need a version for finite boxes that is implicitly contained in [5] and explicitly stated in [6]:

Theorem 2.2 (Lower bound in a finite box). *For a positive potential v with finite range there is a $\delta > 0$ such that*

$$E_0(N,L)/N \geq 4\pi\mu\rho a\left(1 - C\,Y^{1/17}\right) \tag{2.5}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are constants, independent of N and L. (Note that the condition on L/a requires in particular that N must be large enough, $N > (\mathrm{const.})Y^{-1/17}$.)

These results are stated for interactions of finite range. An extension to potentials v of infinite range decreasing faster than $1/r^3$ at infinity is obtained by approximating v by finite range potentials, controlling the change of the scattering length as the cut-off is removed. In this case the estimate holds also, but possibly with an exponent different from 1/17 and a different constant. It should be noted, however, that the form of the error term in (2.4) is dictated by the method of proof. The true error term presumably does not have a negative sign for sufficiently small Y.

3 An upper bound for the QM energy

We now turn to the inhomogeneous gas. In order to prove Eq. (1.15) one has to establish upper and lower bounds for E^{QM} in terms of E^{GP} with errors that vanish in the limit considered. As usual, the upper bound is easier. It is based on test wave functions of the form

$$\Psi(\vec{x}_1,\ldots,\vec{x}_N) = \prod_{i=1}^{N} \Phi^{\mathrm{GP}}(\vec{x}_i) F(\vec{x}_1,\ldots,\vec{x}_N). \tag{3.1}$$

where F is constructed in the following way:

$$F(\vec{x}_1,\ldots,\vec{x}_N) = \prod_{i=1}^{N} f(t_i(\vec{x}_1,\ldots,\vec{x}_i)), \tag{3.2}$$

where $t_i = \min\{|\vec{x}_i - \vec{x}_j|, 1 \le j \le i-1\}$ is the distance of $\vec{x}_i$ to its *nearest neighbor* among the points $\vec{x}_1,\ldots,\vec{x}_{i-1}$ and f is a function of $t \ge 0$. With u_0 the zero energy scattering solution and $f_0(r) = u_0(r)/r$ the function f can be taken as

$$f(r) = f_0(r)/f_0(b) \tag{3.3}$$

for $r < b \equiv (4\pi\bar{\rho}/3)^{-1/3}$ and 1 otherwise. The function (3.1) is not totally symmetric, but for an upper bound it is nevertheless an acceptable test wave function since the bosonic ground state energy is equal to the *absolute* ground state energy.

The result of a somewhat lengthy computation is the upper bound

$$E^{\mathrm{QM}} \le E^{\mathrm{GP}}(1 + O(\bar{Y}^{1/3})) \tag{3.4}$$

with $\bar{Y} = 4\pi a^3\bar{\rho}/3$. Note that $\bar{Y} \sim N^{-2}$ since $a \sim N^{-1}$ and $\bar{\rho} \sim N$.

4 The lower bound

To obtain a lower bound for the QM energy in an external potential the strategy is to divide space into boxes and use the estimate (2.5) for a homogeneous gas in each box with *Neumann* boundary conditions. One then minimizes over all possible divisions of the particles among the different boxes, This gives a lower bound to the energy because discontinuous wave functions for the quadratic form defined by the Hamiltonian are now allowed. Finally, one lets the box size tend to zero. However, it is not possible to simply approximate V by a constant potential in each box. To see this consider the case of noninteracting particles, i.e., $v = 0$ and hence $a = 0$. Here $E^{\mathrm{QM}} = N\hbar\omega$, but a 'naive' box method gives only 0 as lower bound, since it clearly pays to put all the particles with a constant wave function in the box with the lowest value of V.

For this reason we start by separating out the GP wave function in each variable and write a general wave function Ψ as

$$\Psi(\vec{x}_1,\ldots,\vec{x}_N) = \prod_{i=1}^{N} \Phi^{\mathrm{GP}}(\vec{x}_i) F(\vec{x}_1,\ldots,\vec{x}_N) \tag{4.1}$$

This defines F for a given Ψ because $\Phi^{\rm GP}$ is everywhere strictly positive, being the ground state of the operator $-\Delta+V+8\pi a|\Phi^{\rm GP}|^2$. We now compute the expectation value of H in the state Ψ, using partial integration and the variational equation (1.2) for $\Phi^{\rm GP}$. The result is

$$\frac{\langle\Psi,H\Psi\rangle}{\langle\Psi,\Psi\rangle}-E^{\rm GP}=4\pi a\bar{\rho}N+Q(F) \tag{4.2}$$

with

$$Q(F)=\sum_{i=1}^N\frac{\int\prod_{k=1}^N\rho^{\rm GP}(\vec{x}_k)\left(|\nabla_i F|^2+\sum\limits_{j=1}^{i-1}v(|\vec{x}_i-\vec{x}_j|)|F|^2-8\pi a\rho^{\rm GP}(\vec{x}_i)|F|^2\right)}{\int\prod_{k=1}^N\rho^{\rm GP}(\vec{x}_k)|F|^2}. \tag{4.3}$$

Compared to the expression for the energy involving Ψ itself we have thus obtained the following replacements:

$$V(\vec{x})\to-8\pi a\rho^{\rm GP}(\vec{x}),\quad\text{and}\quad\prod_{i=1}^N d\vec{x}_i\to\prod_{i=1}^N\rho^{\rm GP}(\vec{x}_i)d\vec{x}_i. \tag{4.4}$$

(Recall that $\rho^{\rm GP}(\vec{x})=|\Phi^{\rm GP}(\vec{x})|^2$.) We have to show that the normalized quadratic form Q is bounded below by $-4\pi a\bar{\rho}N$, up to small errors, and we use the box method on *this* problem.

Labeling the boxes by an index α we have

$$\inf_F Q(F)\geq\inf_{\{n_\alpha\}}\sum_\alpha\inf_{F_\alpha}Q_\alpha(F_\alpha), \tag{4.5}$$

where Q_α is defined by the same formula as Q but with the integrations limited to the box α, F_α is a wave function with particle number n_α, and the infimum is taken over all distributions of the particles with $\sum n_\alpha=N$. We now want to use (2.5) and therefore we must approximate $\rho^{\rm GP}$ by a constant in each box. Let $\rho_{\alpha,\rm max}$ and $\rho_{\alpha,\rm min}$, respectively, denote the maximal and minimal values of $\rho^{\rm GP}$ in box α. We obtain

$$Q_\alpha(F_\alpha)\geq\frac{\rho_{\alpha,\rm min}}{\rho_{\alpha,\rm max}}E_0(n_\alpha,L)-8\pi a\rho_{\alpha,\rm max}n_\alpha, \tag{4.6}$$

where L is the side length of each box and $E_0(n,L)$ is the ground state energy of n bosons in a box without external potential. Now by Theorem 1.1 $E_0(n_\alpha,L)\approx 4\pi a n_\alpha^2/L^3$, and

$$\inf_{\{n_\alpha\}}\sum_\alpha(4\pi n_\alpha^2/L^3-8\pi\rho_{\alpha,\rm max}n_\alpha)\geq-4\pi\sum_\alpha\rho_{\alpha,\rm max}^2L^3\approx-4\pi\int\left(\rho^{\rm GP}\right)^2=-4\pi\bar{\rho}N, \tag{4.7}$$

which looks promising, were it not for the factor $\rho_{\alpha,\min}/\rho_{\alpha,\max}$ in (4.6) which we would like to replace by 1 for small boxes. The problem is that for any fixed size of boxes $\rho_{\alpha,\min}/\rho_{\alpha,\max}$ tends rapidly to zero for boxes far from the origin.

This problem can be solved by enclosing the whole system in a big box Λ_R of side length R. If $\Phi_R^{\rm GP}$ is the solution of the GP equation with Neumann conditions on the boundary of Λ_R (this is the minimizer of a GP functional where the integration is restricted to Λ_R), then $\rho_R^{\rm GP} = |\Phi_R^{\rm GP}|^2$ is bounded from below away from zero in Λ_R. Replacing in (4.3) everywhere $\rho^{\rm GP}$ by $\rho_R^{\rm GP}$ and restricting the integrations to Λ_R we can let the side lengths of the small boxes tend to zero and be sure that $\rho_{\alpha,\min}/\rho_{\alpha,\max} \to 1$ uniformly for all the small boxes.

For this method to work, however, we must control the error made by enclosing the system in the big box. Let $E_R^{\rm QM}(N,a)$ denote the quantum mechanical ground state energy in Λ_R with Neumann conditions on the boundary. The essential step is

Lemma 4.1. *There is an $R_0 < \infty$, depending only on Na such that*

$$E^{\rm QM}(N,a) \geq E_R^{\rm QM}(N,a) \tag{4.8}$$

for all $R \geq R_0$ and all N, a with Na fixed.

This lemma follows from $V(\vec{x}) \to \infty$ for $|\vec{x}| \to \infty$, together with an estimate for the chemical potential from above:

$$E_R^{\rm QM}(N+1,a) - E_R^{\rm QM}(N,a) \leq e(Na)(1 + O(\bar{Y}^{1/3})) \tag{4.9}$$

where $e(Na)$ depends only on Na and is independent of R. The proof of (4.9) is similar to the proof of the upper bound (3.4) but this time one uses

$$\Psi_0^N(\vec{x}_1,\ldots,\vec{x}_N) f(t_{N+1}) \tag{4.10}$$

with Ψ_0^N the ground state wave function for N-particles and f as in (3.3) as a test wave function for the $N+1$-particle Hamiltonian. Besides the lemma one needs the easy to verify fact that the GP energy $E_R^{\rm GP}$ in the box Λ_R converges to $E^{\rm GP}$ as $R \to \infty$.

The lower bound, and hence the main result, now follows from a rigorous version of (4.7) in the box Λ_R. We use (2.5) in the boxes α; the error here is $O(Y_\alpha^{1/17})$ with $Y_\alpha \sim a^3 n_\alpha / L^3 \leq a^3 N/L^3$. For Na fixed, this is $O(N^{-2/17}L^{-3/17})$. The difference between $\rho_{\alpha,\max}$ and $\rho_{\alpha,\min}$ introduces an additional error, $O(L)$. Both error terms are of the same order for $N \to \infty$ if we choose $L \sim N^{-1/10}$. We thus obtain

$$E^{\rm QM}(N,a) \geq E_R^{\rm QM}(N,a) \geq E_R^{\rm GP}(N,a)(1 - ({\rm const.})N^{-1/10}). \tag{4.11}$$

The constant may depend on R, but this is of no harm, since we first take $N \to \infty$ and then $R \to \infty$, using $E_R^{\rm GP} \to E^{\rm GP}$ and (1.13). This proves (1.15). Convergence of the densities, (1.16), is obtained in a standard way (see, e.g., [8]) by variation with respect to the external potential.

5 Concluding remarks

Bose Einstein condensation in the ground state is a concept that involves the full one particle density matrix

$$\gamma_N(\vec{x}, \vec{x}') = N \int \Psi_0(\vec{x}, \vec{x}_2, \ldots, \vec{x}_N)^* \Psi_0(\vec{x}', \vec{x}_2, \ldots, \vec{x}_N) d\vec{x}_2 \cdots d\vec{x}_N \tag{5.1}$$

and not only its diagonal, $\rho^{\rm QM}(\vec{x}) = \gamma_N(\vec{x}, \vec{x})$ considered here. Expressed in terms of creation and annihilation operators we can also write

$$\gamma_N(\vec{x}, \vec{x}') = \langle a^*(\vec{x}) a(\vec{x}')\rangle_0, \tag{5.2}$$

with $\langle\cdot\rangle_0$ the expectation value in the ground state. As an integral kernel, γ_N is a positive trace class operator. If N_0 denotes its largest eigenvalue BE condensation means that there is a constant $c > 0$ so that

$$N_0 > cN \tag{5.3}$$

for all N. This definition applies also if $\langle\cdot\rangle_0$ is replaced by a thermal equilibrium state at nonzero temperature.

Note that the density in momentum space is

$$\langle \tilde{a}^*(\vec{p}) \tilde{a}(\vec{p})\rangle_0 = \int \exp(i\vec{p}\cdot(\vec{x} - \vec{x}')) \gamma_N(\vec{x}, \vec{x}') d\vec{x} d\vec{x}' \ , \tag{5.4}$$

and this differs from $\left| \int \exp(i\vec{p}\cdot\vec{x}) \sqrt{\rho(\vec{x})} d\vec{x} \right|^2$ unless γ_N has rank 1.

It is often claimed that $\Phi^{\rm GP}$ is (approximately) the eigenfunction to the highest eigenvalue of $\gamma_N(\vec{x}, \vec{x}')$ and hence that $|\tilde{\Phi}^{\rm GP}(\vec{p})|^2$ gives the momentum distribution of the condensate, but this is not proved yet. In fact, so far the only cases with genuine interaction where BE condensation has been rigorously established in the ground state are lattice gases at precisely half filling. (The hard core lattice Bose gas corresponds to the XY spin 1/2 model and BE condensation was proved in dimension ≥ 3 [12] and dimension 2 [13]. The hard core lattice gas with nearest neighbor repulsion corresponds to the Heisenberg antiferromagnet and condensation was proved for high dimension in [12] and dimension ≥ 3 in [14]. Dimension 2 is still open.)

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