The Gross-Pitaevskii Equation
and the Quantum Many-Body Problem

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0. Introduction

Gross-Pitaevskii Equation for systems with short range interactions:

Stationary:

\[-\Delta \varphi(x) + 2g|\varphi(x)|^2\varphi(x) = \mu \varphi(x),\]

Time-dependent:

\[i \partial_t \psi(x,t) = -\Delta \psi(x,t) + 2g|\psi(x,t)|^2\psi(x,t),\]

\[x \in \mathbb{R}^d, \ d = 1, 2, 3.\]

For \(d = 2, 3\) also of interest to consider Rotating systems:

\[-\Delta \rightarrow (i \nabla + A(x))^2\]

with \(A(x) = \frac{1}{2} \Omega \wedge x.\)
In these lectures the following questions will be discussed:

- What is the meaning of $\varphi(x)$ resp. $\psi(x,t)$ in the many-body context?

- How can the GP equation be rigorously derived, starting from the full many-body Hamiltonian?

The focus will be on the stationary situation, in fact on the ground state.

Main reference:
1. The General Setting

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

$$H_N = \sum_{i=1}^{N} (-\Delta_i + V(x_i)) + \sum_{1 \leq i < j \leq N} v(x_i - x_j).$$

Here $x_i \in \mathbb{R}^3$, $i = 1, \ldots, N$ are the positions of the particles.

More generally, the Laplacian $-\Delta$ can be replaced by $(i\nabla + A(x))^2$, where $A(x)$ is a vector potential.

For the mathematical results we shall assume that $v$ is non-negative and spherically symmetric. Moreover, $V(x) \to \infty$ for $|x| \to \infty$. 
The Hamiltonian operates on symmetric wave functions in $L^2(\mathbb{R}^{3N}, dx_1 \cdots dx_N)$ as is appropriate for (spinless) bosons. For ultracold bosons the normalized ground state wave function $\Psi_0(x_1, \ldots, x_N)$ of $H_N$ is of particular interest.

The particle density associated with a general $N$-particle wave function $\Psi$ is

$$\rho(x) = N \int_{\mathbb{R}^{3(N-1)}} |\Psi(x, x_2, \ldots, x_N)|^2 dx_2 \cdots dx_N$$

and the one-particle density matrix is

$$\rho^{(1)}(x, x') = N \int_{\mathbb{R}^{3(N-1)}} \Psi(x, x_2, \ldots, x_N) \Psi^*(x', x_2, \ldots, x_N) dx_2 \cdots dx_N .$$

The latter is the kernel of a positive trace-class operator with trace $N$. This can be generalized also to mixed states.
2. The Concept of BEC for an Interacting Gas

General idea: BEC means “macroscopic occupation of a single one-particle state”. If there was no interaction, i.e., $v \equiv 0$, the many-body ground state $\Psi_0$ of $H_N$ would have the form $\psi_0 \otimes^N$ with $\psi_0$ the ground state of the one-particle operator $-\Delta + V$. BEC trivially holds for such a state. It is, however, a nontrivial question whether BEC holds for thermal equilibrium states at positive temperatures. That this is so far an ideal Bose gas in the thermodynamic limit and $d = 3$ was discovered by Albert Einstein in 1924.

For interacting bosons the question is nontrivial even at temperature zero, i.e., in the many-particle ground state!
**Precise definition:** Let $\varphi$ be a single-particle wave function and denote the projector onto $\varphi$ by $P_{\varphi}$. Then the average occupation of $\varphi$ in an $N$-particle state $\langle \cdot \rangle$ (that can be pure or mixed) is

$$N_\varphi = \langle P_{\varphi} \otimes 1 \otimes 1 \cdots + 1 \otimes P_{\varphi} \otimes 1 \cdots \rangle.$$

In terms of creation and annihilation operators this can alternatively be written as

$$N_\varphi = \langle a(\varphi)^\dagger a(\varphi) \rangle.$$

BEC in the state $\langle \cdot \rangle$ means that for some 1-particle state $\varphi$,

$$N_\varphi = O(N).$$

for $N \to \infty$, more precisely,

$$N_\varphi/N \geq c > 0$$

for all (large enough) $N$. 


In terms of the one-particle density matrix \( \rho^{(1)}(x, x') = \langle a(x)^\dagger a(x') \rangle \) we can also write

\[
N_\varphi = \int \int \varphi(x)^* \rho^{(1)}(x, x') \varphi(x') \, dx \, dx'.
\]

The density matrix has a spectral decomposition:

\[
\rho^{(1)}(x, x') = \sum_i \lambda_i \varphi_i(x) \varphi_i^*(x')
\]

with \( \lambda_0 \geq \lambda_1 \geq \ldots \) and orthonormal \( \varphi_i \). Because \( N_{\varphi_0} = \lambda_0 \) is the maximal occupancy of any single-particle state, BEC in the many-body state to which \( \rho^{(1)}(x, x') \) corresponds means that

\[
\lambda_0 = O(N).
\]

The eigenfunction \( \varphi_0(x) \) to the highest eigenvalue of \( \rho^{(1)}(x, x') \) is often referred to as the wave function of the condensate.
Note that
\[ \lambda_0 |\varphi_0(x)|^2 \quad \text{resp.} \quad \lambda_0 |\tilde{\varphi}_0(p)|^2 \]

is the spatial density resp. the momentum density of the condensate. For homogeneous gases in a large box \( \Lambda \) the wave function of the condensate can be expected to be constant, i.e., \( \varphi_0 = |\Lambda|^{-1/2} \). Since
\[ \lambda_0 = \int \int \varphi_0^*(x) \rho^{(1)}(x, x') \varphi_0(x') dx dx' , \]
BEC for a homogeneous gas means
\[ |\Lambda|^{-1} \int \int \rho^{(1)}(x, x') dx dx' = O(N) \tag{3} \]

instead of \( o(N) \) if there is no BEC. This is called "Off Diagonal Long Range Order" (ODLRO).
IMPORTANT REMARK: To make the definition of BEC precise, the $N$ dependence of $\Lambda$, or more generally, the $N$ dependence of the parameters of the external potential $V$, has to be specified! Important cases are:

- **Thermodynamic limit:** $N \to \infty$, $|\Lambda| \to \infty$, $N/|\Lambda| = \text{const.}$

- **Gross-Pitaevskii-limit:** $N \to \infty$, $Na/L = \text{const.}$ with $a$ the *scattering length* of $v$ and $L$ the length scale associated with $-\Delta + V$.

- **‘Thomas-Fermi’-limit:** $N \to \infty$, $Na/L \to \infty$, but $Na^3/L^3 \to 0$. 
3. The Ground State Energy

3.1 The Scattering Length
Consider a spherically symmetric pair interaction potential $v$ of short range. The zero energy scattering equation is

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

Writing $\psi(x) = u(r)/r$ with $r = |x|$ this is equivalent to

$$-u''(r) + \frac{1}{2}v(r)u(r) = 0.$$ 

For $r$ larger than the range of $v$ the solution with $u(0) = 0$ has the form

$$u(r) = (\text{const.})(r - a)$$

with a constant $a$ that is called the scattering length of $v$. 
Equivalently,

\[ a = \lim_{r \to \infty} \left[ r - \frac{u(r)}{u'(r)} \right]. \]

For \( \psi(x) = u(r)/r \) we have

\[ \psi(x) = (\text{const.}) \left( 1 - \frac{a}{r} \right). \]

If \( v \geq 0 \), then also \( a \geq 0 \), but \( a \leq \text{range of } v \).

For a hard sphere potential \( a = \text{radius of the hard sphere} \).

If \( v \) is not positive then \( a \) can be negative. If \( -\Delta + \frac{1}{2}v \) has bound states, then \( a \) can be much larger than the range of \( v \).
If \( v \geq 0 \) the scattering length determines completely the ground state energy \( E_0(2, L) \) of a pair of Bosons in a large box \( \Lambda \) of side length \( L \gg a \).

\[
E_0(2, \Lambda) \approx \frac{8 \pi a}{L^3}
\]

### 3.2 The GSE of a dilute gas

Consider now for \( v \geq 0 \) the Hamiltonian of \( N \) Bosons in a box \( \Lambda \) of side length \( L \) with appropriate boundary conditions:

\[
H_N = -\sum_{i=1}^{N} \Delta^2_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j)
\]

Ground state energy:

\[
E_0(N, L) = \inf_{\|\psi\|=1} \langle \psi, H_N \psi \rangle.
\]
Energy per particle in thermodynamic limit, $\rho = N/L^3$ fixed:

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

Ask for the low density asymptotics of $e_0(\rho)$. Low density means

$$a \ll \rho^{-1/3}$$

i.e., the scattering length is much smaller than the mean particle distance. This can also be written as $\rho a^3 \ll 1$. The basic formula for the energy is

**THEOREM** (GSE of a dilute gas): *For* $\rho a^3 \ll 1$

$$e_0(\rho) = 4\pi a \rho (1 + o(1))$$
Heuristic argument for the formula:

"For a dilute gas only two body scattering matters", so

\[ E_0(N, L) \approx \frac{N(N-1)}{2} E_0(2, L) \approx \frac{N^2 8\pi a}{2 L^3} \approx N 4\pi a \rho. \]

This heuristic argument is, however, very far from a rigorous proof and it gives a wrong answer in two dimensions!

The formula has an interesting history and it took almost 70 years to establish it rigorously. (Lenz (1929), Bogoliubov (1947), Huang, Yang,..., Lieb (50’s and 60’s), Dyson 1957, Lieb, JY 1998.)

A rigorous upper bound was given by Dyson in 1957 but an asymptotically correct lower bound (Lieb, JY) was not obtained until 40 years later.
Why is the lower bound so difficult?

If \( \rho \) is small, then \( e_0(\rho) \) is small. Distinguish two regimes:


2. “Soft potential”, \( v \) small. Energy mostly potential. Lowest order perturbation theory (with the uncorrelated, unperturbed state \( \Psi_0 = L^{-3N/2} \)) gives

\[
e_0(\rho) \approx \frac{1}{2} \rho \int v(x) d^3x
\]

Wrong answer (independent of \( \hbar \) and \( m! \)), but at least the first Born approximation to \( 4\pi a\rho \). (Note: \( a \) depends on \( \hbar \) and \( m \).)
The g.s.e. does not distinguish the two regimes. Does BEC?

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 by LY and the following lemma is a key element for the lower bound as well as for much of the subsequent developments, in particular the rigorous derivation, by LY and Seiringer, of the GP equation.

**LEMMA (Dyson’s Lemma):** Let $v(r) \geq 0$ with finite range $R_0$. Let $U(r) \geq 0$ satisfy $\int U(r)r^2dr \leq 1$, $U(r) = 0$ for $r < R_0$. Then for all $\psi$ and domains $\mathcal{B} \subset \mathbb{R}^3$ that are star shaped w.r.t. 0

$$\int_{\mathcal{B}} \left[ |\nabla \psi|^2 + \frac{1}{2} v|\psi|^2 \right] \geq a \int_{\mathcal{B} \cap \text{supp} U} U|\psi|^2 + \int_{\mathcal{B} \setminus \text{supp} U} |\nabla \psi|^2$$
4. Gross-Pitaevskii Theory

Consider now the $N$-body Hamiltonian with an external Potential $V$, representing a confining trap:

$$H_N = \sum_{i=1}^{N} \{-\Delta_i + V(x_i)\} + \sum_{1\leq i<j\leq N} v(|x_i - x_j|).$$

The external potential comes with a natural length scale $L_{osc} = \omega^{-1/2}$ where $\omega$ is the spectral gap of $-\Delta + V$.

One would like to study the ground state properties of $H$, and in particular BEC, in the Gross-Pitaevskii (GP) limit where $N \to \infty$ with a fixed value of the GP interaction parameter

$$g \equiv 4\pi Na/L_{osc} = e_0(\rho)/\omega.$$ 

with $\rho = N/L_{osc}^3$. 

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Note: \( \rho a^3 \sim g/N^2 = O(1/N^2) \) if \( g \) is fixed, so the GP limit is a special case of a dilute limit.

The GP limit can be achieved either by keeping \( a \) fixed and scaling the external potential \( V \) so that \( L_{\text{osc}} \sim N \), or, by keeping \( V \) fixed and taking \( a \sim N^{-1} \). The latter can formally be regarded as a scaling of the interaction potential:

\[
v(r) = N^2 v_1(Nr)
\]

Important point: 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 from the many-body Hamiltonian is very different from mean field techniques.
It turns out that in the GP limit the ground state can be described by minimizing a functional of functions on $\mathbb{R}^3$, the GP energy functional

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

with the subsidiary condition $\int |\varphi|^2 = 1$.

**Motivation** for the term $g|\varphi|^4$: With $\rho(x) = N|\varphi(x)|^2$ the local density, we have

$$ Ng \int |\varphi|^4 = 4\pi a \int \rho(x)^2, $$

and $4\pi a \rho(x)^2$ is the interaction energy per unit volume.
The minimizer of the GP functional is the unique, nonnegative solution of the (time independent) Gross-Pitaevskii equation

\[ (-\Delta + V + 2g|\varphi|^2)\varphi = \mu \varphi \]

with a Lagrange multiplier $\mu$.

We denote the minimizer by $\varphi^{\text{GP}}(x)$. The corresponding energy is

\[ E_{g}^{\text{GP}} = \mathcal{E}^{\text{GP}}[\varphi^{\text{GP}}] = \inf\{\mathcal{E}^{\text{GP}}[\varphi] : \int |\varphi|^2 = 1\}. \]
The GP energy functional can be obtained formally from the many body Hamiltonian by replacing \( v(x_i - x_j) \) by \( 8\pi a \delta(x_i - x_j) \) and making a Hartree type product ansatz for the many body wave function, i.e., writing

\[
\Psi(x_1, \ldots, x_N) = \varphi(x_1) \cdots \varphi(x_N).
\]

This is not a proof, however, and the true ground state is not of this form. In particular, if \( v \) is a hard sphere potential, \( \langle \Psi, H \Psi \rangle = \infty \) for all such wave functions. Finite energy can in this case only be obtained for functions of the form

\[
\Psi(x_1, \ldots, x_N) = \varphi(x_1) \cdots \varphi(x_N) F(x_1, \ldots, x_N)
\]

with \( F(x_1, \ldots, x_N) = 0 \) if \( |x_i - x_j| \leq a \) for some \( i \neq j \). The upper bound on the energy is, in fact, proved by using trial functions of this form with a judiciously chosen \( F \) involving the zero-energy scattering solution of the two-body problem.
Basic results in GP theory are the following *rigorous* theorems:

**THEOREM (Energy asymptotics)** If $N \to \infty$ with $g$ fixed, then

$$\frac{E_0(N,a)}{NE_{g,G}} \to 1$$

**THEOREM (BEC in GP limit)** If $N \to \infty$ with $g$ fixed (i.e., $a \sim N^{-1}L_{osc}$), then

$$\frac{1}{N}\rho^{(1)}(x,x') \to \varphi^{GP}(x)\varphi^{GP}(x').$$

In other words: There is complete BEC in the GP limit and the solution of the GP equation is the wave function of the condensate.

**COROLLARY:** In the GP limit the normalized particle density in the many-body ground state converges to $N|\varphi^{GP}(x)|^2$ and the momentum density to $N|\tilde{\varphi}^{GP}(p)|^2$. 

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GP density compared to measured density and density without interaction
Emergence of BEC in a trap
It is instructive to consider the properties of $\varphi^{\text{GP}}$ as the interaction parameter $g$ varies, in particular the limiting case $g \gg 1$.

Assume $V$ is a homogeneous function of some order $s > 1$, i.e., $V(\lambda x) = \lambda^s V(x)$.

**Heuristic considerations:** Let $R$ be the spatial extension of the condensate. Then $|\varphi|^2 \sim R^{-3}$ and the three terms in the GP energy functional are of the following orders of magnitude:

- $\int |\nabla \varphi|^2 \sim R^{-2}$
- $\int V|\varphi|^2 \sim R^s$
- $g \int |\varphi|^4 \sim gR^{-3}$
For $g$ large the minimum of $R^{-2} + R^s + gR^{-3}$ is obtained for

$$R \sim g^{1/(s+3)}$$

In particular for $s = 2$ (quadratic trap): $R \sim g^{1/5}$.

Note that $\int |\nabla \varphi|^2 \sim R^{-2} \sim g^{-2/(s+3)}$ but the other terms are $\sim g^s/(s+3)$. Hence the kinetic term becomes irrelevant for $g \gg 1$.

More precisely, writing $x = g^{1/(s+3)}x'$ we obtain

$$E^{\text{GP}}[\varphi] = \frac{gs}{(s+3)} \int_{\mathbb{R}^3} \left( g^{-(s+2)/(s+3)}|\nabla \varphi'|^2 + V|\varphi'|^2 + |\varphi'|^4 \right) dx'$$

with $\varphi'(x') = g^{3/2(s+3)}\varphi(x)$. 
Denoting $|\varphi'(x')|^2$ by $\rho(x')$ we see that in the limit $g \to \infty$ the GP functional simplifies to the so-called ‘Thomas-Fermi functional’

$$\mathcal{E}^{\text{TF}}[\rho] = \int_{\mathbb{R}^3} (V\rho + \rho^2)$$

with normalization $\int \rho = 1$.

The minimizer can be explicitly displayed:

$$\rho^{\text{TF}}(x) = 2[\mu^{\text{TF}} - V(x)]_+$$

where $\mu^{\text{TF}}$ is chosen so that the normalization condition is fulfilled. The minimizer and the ground state energy can be derived rigorously from the many-body problem under the additional hypothesis that the gas stays dilute (TF-Limit). But BEC is not yet proved in this limit, only in the GP limit where $g$ stays fixed!
5. Proof of BEC in the GP Limit

The proof of BEC for trapped, dilute gases (Lieb, Seiringer, 2001) has two *main ingredients*:

One is a refinement of the energy estimates obtained by LY (1998). It shows that the *kinetic energy density* in the ground state is *concentrated in a region in configuration space where two particles are close together*.

The other is an extension of a classical *Poincaré inequality* that estimates an $L_p$ norm of the average value of a function by an $L_q$ norm of its gradient.
Sketch of the proof in a box $\Lambda$ of side length $L$:

Notation: $X = (x_2, \ldots, x_N)$, $\psi_X(x) = \Psi_0(x, X)$. The depletion of the condensate (with the constant wave function $\varphi_0 \equiv L^{-3/2}$) is

$$1 - N_0/N = 1 - (NL^3)^{-1} \int \int \rho^{(1)}(x, x') dx dx' = \int dX \|\psi_X - \langle \psi_X \rangle\|^2$$

where $\langle f \rangle = L^{-3} \int f$.

Simple Poincaré inequality:

$$\|f - \langle f \rangle\|^2 \leq CL^2 \|\nabla f\|^2$$

Generalized Poincaré inequality for $\Omega \subset \Lambda$:

$$\|f - \langle f \rangle\|^2 \leq C_1 L^2 \|\nabla f\|_{L^2(\Omega)}^2 + C_2 |\Omega^c|^{2/3} \|\nabla f\|^2.$$
Localization of the kinetic energy:

While

\[ T_{\text{kin}} \equiv \int dX \| \nabla \psi_X \|^2 \sim \rho a (1 + o(1)) \]

there is an \( \Omega \subset \Lambda \) such that \( |\Omega^c| = L^3 \times o(1) \) and

\[ (\rho a)^{-1} \int dX \| \nabla \psi_X \|^2_{L^2(\Omega)} = o(1). \]

(For the proof of this the technique of Dyson’s Lemma is essential.) Hence, if \( N \to \infty \) with \( g = Na/L \) fixed,

\[ 1 - N_0/N \leq L^2 \rho a \times o(1) = \frac{Na}{L} \times o(1) \to 0 \]

i.e., we have complete BEC in the GP limit.
6. Conclusions and Remarks

1. The GP minimizer $\varphi^{\text{GP}}$, that fulfills the time-independent GP equation, has, in the many-body context, the meaning of the wave function of the condensate, i.e., it is the eigenfunction to the largest eigenvalue of the one-particle density matrix corresponding to the many-body ground state. The GP energy is asymptotically equal to the many-body ground state energy per particle.

2. The derivation of the time-dependent GP equation (Erdős, Schlein, Yau) requires entirely different techniques. For a review see: Benjamin Schlein, *Derivation of Effective Evolution Equations from Microscopic Quantum Dynamics*, ArXiv:0807.4307

3. The time-independent GP equation for rotating systems will be discussed in the last lecture of this minicourse.