Cold Quantum Gases and Bose-Einstein Condensation[*]

Robert Seiringer, McGill University

August 23, 2010

Abstract

Lecture Notes of a course given at the Les Houches summer school "Quantum Theory from Small to Large Scales", August 2–27, 2010.

Contents

1 Quantum Many-Body Systems

1.1 The Hamiltonian

For a system of N particles, the Hamiltonian typically takes the form

$$H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + V(x_1, \ldots x_N)$$

where m_i is the mass of particle i, $p_i \in \mathbb{R}^3$ and $x_i \in \mathbb{R}^3$ are its momentum and position, respectively, and V denotes the total potential energy. Classically, H is a function on phase space, but in quantum mechanics it becomes a linear operator with the substitution $p_j = -i\hbar\nabla_j$. We shall choose units such that $\hbar = 1$ from now on.

The Hamiltonian H_N is a linear operator on Hilbert space, which is a suitable subspace of $L^2(\mathbb{R}^{3N})$, the square integrable functions of N variables $x_i \in \mathbb{R}^3$. Only a subspace is relevant physically, since for two identical bosons, say i and j, there is the symmetry requirement

$$\psi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = \psi(x_1, \ldots, x_j, \ldots, x_i, \ldots x_N)$$

For fermions, there is an additional minus sign, i.e., the wave function is antisymmetric with respect to exchange of coordinates. For simplicity of notation, we ignore here internal degrees of freedom of the particles, like spin, but these could easily be taken into account by adding to the coordinates x_i these additional parameters.

The form of the potential energy depends on the physical system under consideration. Typically, it is a sum of various terms, containing one-particle potentials of the form $\sum_i W(x_i)$, corresponding to an external force, two-body interaction potentials $\sum_{i<j} W(x_i, x_j)$ for pairwise interaction, or even some more complicated interactions involving more than two particles at the same time. We will usually assume that

$$V(x_i, \ldots, x_N) = \sum_{i=1}^{N} W(x_i) + \sum_{1 \leq i < j \leq N} v(|x_i - x_j|).$$

2

1.2 Quantities of Interest

Given the Hamiltonian H_N of a quantum systems, there are many questions one can try to address. The first one might be concerning its ground state energy, i.e., the lowest values of the spectrum, which we denote by

$$E_0(N) = \inf \operatorname{spec} H_N$$

If $E_0(N)$ is an eigenvalue, the corresponding ground state wave function ψ_0 is determined by Schrödinger's equation $H_N \psi_0 = E_0(N)\psi_0$.

More generally, if the system is at some positive temperature $T > 0$, one would like to compute the free energy of the system, given by

$$F = -T \ln \operatorname{Tr} e^{-H_N/T}$$

We choose units such that Boltzmann's constant equals 1, and small often write $T = 1/\beta$. The trace is over the physical Hilbert space, of course, respecting symmetry constraints arising form the indistinguishability of particles. The equilibrium state at temperature T is the Gibbs state

$$\varrho_\beta = e^{-\beta(H-F)}$$

It is normalized to have $\operatorname{Tr} \varrho_\beta = 1$. For large particle number, it is usually hopeless to try to calculate ϱ_β directly, but one will try to investigate properties of the reduced n-particle density matrices, obtained by taking the partial trace of ϱ_β over $N - n$ variables.

It is often convenient not to fix the particle number N, but rather work in the grand-canonical ensemble, where one takes a certain average over the number of particles in the system. For simplicity, consider a system of just one species of particles. The N-particle Hilbert space, $\mathcal{H}_N$, is then the set of square-integrable functions that are either totally symmetric or antisymmetric under permutations, depending on whether the particles are bosons or fermions.

In the grand-canonical ensembles, one has as Hilbert space the Fock space

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{H}_N$$

Here, $\mathcal{H}_0 = \mathbb{C}$ by definition, and the corresponding vector is called the vacuum vector. As Hamiltonian on Fock space one simply takes

$$H = \bigoplus_{N=0}^{\infty} H_N$$

with H_N the N-particle Hamiltonian. Typically, $H_0 = 0$, i.e., the vacuum has zero energy.

For $\mu \in \mathbb{R}$, the grand canonical potential is defined as

$$J = -T \ln \mathrm{Tr}_{\mathcal{F}} e^{-\beta(H - \mu N)}$$

where N denotes the number operator, i.e,

$$N = \bigoplus_{n=0}^{\infty} n$$

Since H is particle number conserving, we can also write this as

$$J = -T \ln \sum_{N \geq 0} z^N \mathrm{Tr}_{\mathcal{H}_N} e^{-\beta H_N}$$

where $z = e^{\beta \mu}$ is called the fugacity.

The grand-canonical Gibbs state is

$$\varrho_{\beta, \mu} = e^{-\beta(H - \mu N - J)}$$

The chemical potential μ is adjusted to achieve a given average particle number $\langle N \rangle$. The latter equals

$$\langle N \rangle = \mathrm{Tr}\, N \varrho_{\beta, \mu} = -\frac{\partial}{\partial \mu} J$$

1.3 Creation and Annihilation Operators on Fock Space

On Fock space $\mathcal{F}$, a particularly useful concept are the creation and annihilation operators $a^\dagger(f)$ and $a(f)$, with $f \in \mathcal{H}_1$, the one-particle Hilbert space. For any $N \geq 0$, we have

$$a^\dagger(f) : \mathcal{H}_N \to \mathcal{H}_{N+1}$$

i.e., it creates a particle. Likewise, $a(f)$ annihilates a particle, i.e.,

$$a(f) : \mathcal{H}_N \to H_{N-1}$$

Explicitly, they are defined as follows. If ψ_N is an N-particle wave function in $\mathcal{H}_N$,

$$\big(a^\dagger(f)\psi_N\big)(x_1, \ldots, x_{N+1}) = \frac{1}{\sqrt{N+1}} \sum_{i=1}^{N+1} f(x_i)\psi_N(x_1, \ldots, \not{x}_i, \ldots, x_{N+1})$$

and

$$\big(a(f)\psi_N\big)(x_1, \ldots, x_{N-1}) = \sqrt{N} \int_{\mathbb{R}^3} \bar{f}(x_N)\psi_N(x_1, \ldots, x_{N-1}, x_N)dx_N$$

4

This definition works for bosons, for fermions one has to introduce the appropriate (-1) factors to preserve the antisymmetry of the wave functions. One readily checks that these operators satisfy $a(f)^\dagger = a^\dagger(f)$, i.e., $a^\dagger(f)$ is the adjoint of $a(f)$, as well as the canonical (anti-)commutation relations

$$[a(f), a^\dagger(g)] = \langle f|g\rangle \ , \ [a(f), a(g)] = 0 \ , \ [a^\dagger(f), a^\dagger(g)] = 0$$

Here, $[\cdot, \cdot]$ denotes the usual commutator $[A, B] = AB - BA$ for bosons, while it is the anticommutator $[A, B] = AB + BA$ for fermions.

Consider now a typical many-body Hamiltonian containing one- and two-body terms. For h a one-body operator and W a two-body operator, the N-particle Hamiltonian is thus of the form

$$H_N = \sum_{i=1}^{N} h_i + \sum_{1 \leq i < j \leq N} W_{ij}$$

where the subscripts indicate what particles the operator acts on. Using creation and annihilation operators, the Fock space Hamiltonian $H = \bigoplus_{N \geq 0} H_N$ can conveniently be written as

$$H = \sum_{i,j} \langle \varphi_i|h|\varphi_j \rangle \, a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} \langle \varphi_i \otimes \varphi_j|W|\varphi_k \otimes \varphi_l \rangle \, a_i^\dagger a_j^\dagger a_k a_l$$

where $\{\varphi_i\}$ is an orthonormal basis of $\mathcal{H}_1$, and $a_i^\dagger = a^\dagger(\varphi_i)$, $a_i = a(\varphi_i)$. A possible choice of the basis $\{\varphi_i\}$ is to diagonalize h, i.e.,

$$\langle \varphi_i|h|\varphi_j \rangle = e_i \delta_{ij}$$

The number operator N is simply $N = \sum_i a_i^\dagger a_i$.

In terms of the creation and annihilation operators, the reduced n-particle density matrices $\gamma^{(n)}$ of a state on Fock space are defined via the expectation values

$$\langle f_1 \otimes \cdots \otimes f_n|\gamma^{(n)}|g_1 \otimes \cdots \otimes g_n \rangle = \langle a^\dagger(g_1) \ldots a^\dagger(g_n) a(f_n) \ldots a(f_1) \rangle$$

Since product functions span the whole n-particle space, this defines $\gamma^{(n)}$ uniquely. For a state with a fixed particle number, the definition agrees with the previous definition in the canonical ensemble using partial traces (except for an overall normalization factor).

1.4   Ideal Quantum Gases

Consider now an ideal quantum system without interactions. The N-particle Hamiltonian is simply $H_N = \sum_{i=1}^{N} h_i$, where, for example,

$$h = \frac{1}{2m}p^2 = -\frac{1}{2m}\Delta$$

on the cube $[0, L]^3$ with appropriate boundary conditions. In particular, we assume that h has discrete spectrum. Let us denote the eigenvalues of h by e_i,

$$e_0 \leq e_1 \leq e_2 \leq \dots$$

On Fock space, we then have

$$H = \sum_{i \geq 0} e_i a_i^\dagger a_i$$

and also

$$\beta H - \mu N = \sum_{i \geq 0} \varepsilon_i a_i^\dagger a_i$$

with $\varepsilon_i = \beta e_i - \mu$.

We wish to calculate

$$\ln \mathrm{Tr}\, e^{-\sum_i \varepsilon_i a_i^\dagger a_i}$$

The spectrum of $\sum_i \varepsilon_i a_i^\dagger a_i$ is of the form $\sum_i \varepsilon_i n_i$, with $n_i \in \{0, 1, 2, \dots\}$ for bosons, and $n_i \in \{0, 1\}$ for fermions. Summing over all possible occupation numbers is the same as summing over all eigenstates, hence we have

$$\mathrm{Tr}\, e^{-\sum_i \varepsilon_i a_i^\dagger a_i} = \prod_i \sum_n e^{-\varepsilon_i n} = \prod_i \begin{cases} (1 - e^{-\varepsilon_i})^{-1} & \text{bosons} \\ 1 + e^{-\varepsilon_i} & \text{fermions} \end{cases}$$

For bosons, we have to assume that $\varepsilon_i > 0$ for all i for the geometric series to converge. In particular

$$\ln \mathrm{Tr}\, e^{-\sum_i \varepsilon_i a_i^\dagger a_i} = \sum_i \mp \ln(1 \mp e^{-\varepsilon_i})$$

where $-$ is for bosons and $+$ for fermions.

Consider now an ideal gas in a cubic box of side length L, with periodic boundary conditions. The spectrum of $p^2 = -\Delta$ equals

$$\left(\frac{2\pi}{L}\right)^2 \left(n_x^2 + n_y^2 + n_z^2\right)$$

with $(n_x, n_y, n_z) \in \mathbb{Z}^3$. The corresponding eigenstates are the plane waves $e^{ip \cdot x}$, with $p \in (\frac{2\pi}{L}\mathbb{Z})^3$. The grand canonical potential (which equals the negative of the pressure times the volume in this case) thus equals

$$J = \pm T \sum_{p \in (\frac{2\pi}{L}\mathbb{Z})^3} \ln\left(1 \mp e^{-\beta(p^2 - \mu)}\right)$$

where we set the mass of the particles equal to $1/2$ for simplicity.

For bosons, we have to assume that $\mu < 0$. This is not really a restriction, however, as any particle number can be achieved even for negative μ. In fact, the average particle number equals

$$\langle N \rangle = -\frac{\partial}{\partial \mu} J = \sum_{p \in (\frac{2\pi}{L} \mathbb{Z})^3} \underbrace{\frac{1}{e^{\beta(p^2 - \mu)} \mp 1}}_{\langle a_p^\dagger a_p \rangle}$$

Here, the summands are just $\langle a_p^\dagger a_p \rangle$, the average occupation number of momentum p. As μ varies within $(-\infty, 0)$ (for bosons), and $(-\infty, \infty)$ (for fermions), clearly $\langle N \rangle$ various between 0 and $+\infty$.

We now perform a thermodynamic limit $L \to \infty$. The sum over p can then be interpreted as a Riemann sum for the corresponding integral. In fact,

$$\frac{1}{L^3} \sum_{p \in (\frac{2\pi}{L} \mathbb{Z})^3} \longrightarrow \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} dp$$

as $L \to \infty$. The thermodynamic pressure of the system is thus

$$P = -\lim_{L \to \infty} \frac{J}{L^3} = \mp \frac{T}{(2\pi)^3} \int_{\mathbb{R}^3} \ln\left(1 \mp e^{-\beta(p^2 - \mu)}\right) dp$$

and the average density equals

$$\varrho = \lim_{L \to \infty} \frac{\langle N \rangle}{L^3} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{e^{\beta(p^2 - \mu)} \mp 1} dp. \tag{1}$$

Let us know restrict our attention to the bosonic case, where there is a minus sign in the denominator in (1). Notice that the density stays bounded as $\mu \to 0$! I.e.,

$$\varrho_c(\beta) := \lim_{\mu \nearrow 0} \varrho = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{e^{\beta p^2} - 1} dp < \infty \tag{2}$$

since the integrand behaves like $|p|^{-2}$ for small p, which is integrable in 3 dimensions.

What is happening here? Recall that μ has to be chosen as to fix the density ϱ and, hence, has to depend on L, in general. If $\varrho < \varrho_c(\beta)$, then $\mu(L) \to \mu < 0$ in the thermodynamic limit. But when $\varrho \geq \varrho_c(\beta)$, $\mu(L)$ has to tend to zero as $L \to \infty$. In this case, the limits $L \to \infty$ and $\mu \to 0$ must be taken simultaneously and, in particular, do not commute.

In fact, if $\varrho > \varrho_c(\beta)$, then μ is asymptotically equal to

$$\mu = \left(-\beta L^3 (\varrho - \varrho_c(\beta))\right)^{-1} \quad \text{as } L \to \infty$$
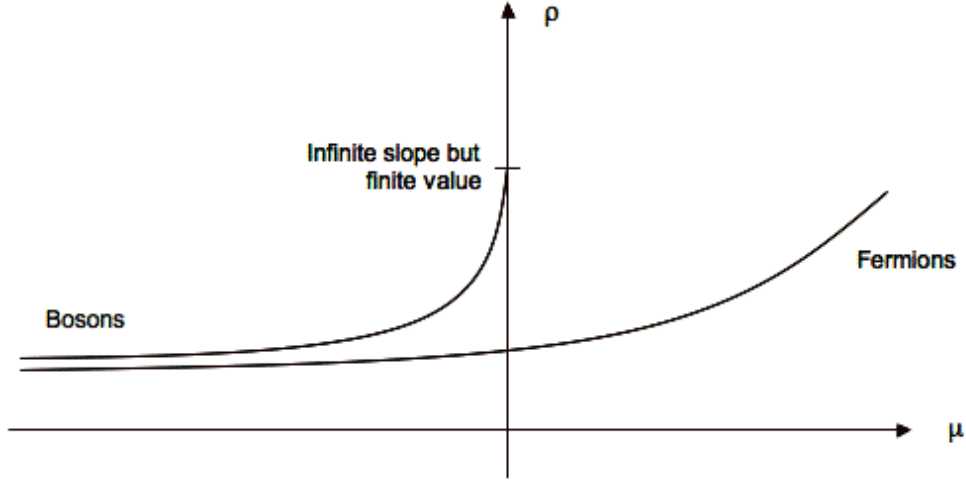
Figure 1: Particle density of an ideal quantum gas at infinite volume, as a function of the chemical potential μ.

For this value of μ, we see that

$$\lim_{L\to\infty} \frac{1}{L^3}\langle a_0^\dagger a_0 \rangle = \lim_{L\to\infty} \frac{1}{L^3}\frac{1}{e^{-\beta\mu}-1} = \varrho - \varrho_c(\beta)$$

That is, the zero momentum state is occupied by a macroscopic fraction of all the particles. This phenomenon is called **Bose-Einstein Condensation** (BEC). It occurs for $\varrho > \varrho_c(\beta)$, i.e., for ϱ bigger than the critical density or, equivalently, for

$$T < T_c(\varrho) = \frac{4\pi}{\zeta}(3/2)^{2/3}\varrho^{2/3}$$

since $\varrho_c(\beta) = \zeta(3/2)(4\pi)^{-3/2}\beta^{-3/2}$. Here, ζ denotes the Riemann zeta functions

$$\zeta(z) = \sum_{k\geq 1} k^{-z}$$

I.e., BEC occurs below a critical temperature $T_c(\varrho)$.

We note that only the zero momentum mode is macroscopically occupied, and the other occupations are much smaller. The smallest positive eigenvalue of the Laplacian equals $(2\pi/L)^2$, and

$$\frac{1}{e^{\beta(2\pi/L)^2}-1} \sim L^2 \ll L^3 \quad \text{for large } L.$$

BEC represents a phase transition in the usual sense, namely that the thermodynamic functions exhibit a non-analytic behavior. Consider, for instance, the free energy, which is given in a standard way

8

as the Legendre transform of the pressure. Specifically, the free energy per unit volume equals

$$f(\beta, \varrho) = \mu \varrho + \frac{T}{(2\pi)^3} \int_{\mathbb{R}^3} \ln\left(1 - e^{-\beta(p^2 - \mu)}\right) dp \qquad (3)$$

where μ is determined by Eq. (1) if $\varrho < \varrho_c(\beta)$, and $\mu = 0$ if $\varrho \geq \varrho_c(\beta)$. In the latter case, we see that $f(\beta, \varrho)$ does not actually depend on ϱ, and is constant for $\varrho > \varrho_c(\beta)$. In particular, f is not analytic. Intuitively, what is happening as one increases the density beyond $\varrho_c(\beta)$ is that all additional particles occupy the zero momentum mode and hence do not contribute to the energy or the entropy, hence also not the the free energy.
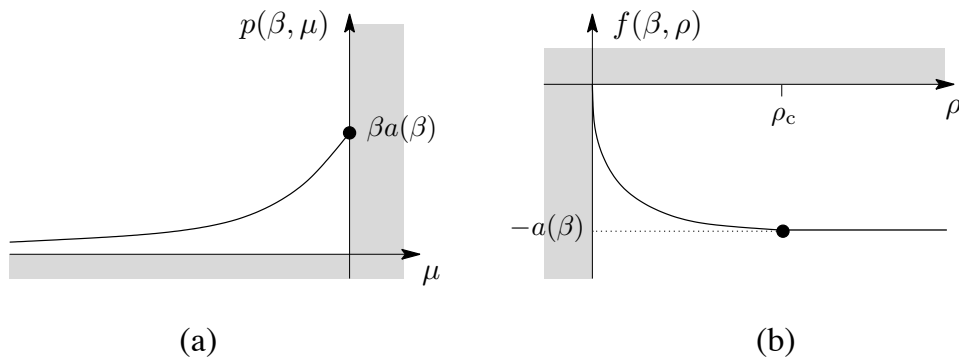

Figure 2: The pressure and the free energy of the ideal Bose gas in three dimensions.

We conclude this section by noting that the grand-canonical ensemble is somewhat unphysical for the ideal Bose gas for $\varrho > \varrho_c(\beta)$, because of large particle number fluctuations. One readily computes that

$$\langle n_p(n_p - 1) \rangle = 2\langle n_p \rangle^2 \qquad (4)$$

for any p, where $n_p = a_p^\dagger a_p$ denotes the number of particles with momentum p. Note that (4) is independent of β and μ. It can be easily checked from the explicit form of the Gibbs state, or follows from Wick's rule, for instance.

The factor 2 on the right side of (4) is crucial. It means that the variance of the occupation number is of the same order is its value. In particular, if there is a macroscopic occupation, also the variance is macroscopic! By summing over p, we also see that

$$\langle N(N - 1) \rangle = \langle N \rangle^2 + \sum_p \langle n_p \rangle^2$$

The last term of is of the order $\langle N \rangle^2$ if and only if $\varrho > \varrho_c(\beta)$. That is, there are macroscopically large particle number fluctuations in this case. For real, interacting systems, such fluctuation will typically be suppressed and this problem is not expected to occur.

The macroscopic particle number fluctuations in particular mean that there is not a full equivalence of ensembles for the ideal Bose gas. Nevertheless, working in the canonical ensemble will produce the same free energy (3) and the same occupation numbers $\langle n_p \rangle$ in the thermodynamic limit. In particular, the conclusion concerning BEC remains the same in the canonical ensemble, although the analysis is much more tedious. (See [2] or also Appendix B of [22].)

2 BEC for Interacting Systems

2.1 The Criterion for BEC

Recall the definition of the one-particle density matrix γ. For $\langle \cdot \rangle$ a state on Fock space,

$$\langle g | \gamma | f \rangle = \langle a^\dagger(f) a(g) \rangle$$

Note that γ is a positive trace class operator on the one-particle Hilbert space $\mathcal{H}_1$, with

$$\mathrm{Tr}\, \gamma = \sum_i \langle \varphi_i | \gamma | \varphi_i \rangle = \left\langle \sum_i a_i^\dagger a_i \right\rangle = \langle N \rangle$$

This definition applies to any state on Fock space, not only thermal equilibrium states. In particular, one can also consider states of definite particle number, and hence recover the definition for the canonical ensemble.

According to a criterion by Penrose and Onsager [17], BEC is said to occur if γ has an eigenvalue of the order of $\langle N \rangle$ of large $\langle N \rangle$. The corresponding eigenfunction is called the **condensate wave function**.

Since this definition involves large particle numbers $\langle N \rangle$, it refers, strictly speaking, not to a single state but rather a sequence of states for larger and larger system size. When one speaks about the occurrence of BEC one hence always has to specify how various parameters depend on this size.

The standard case where one would like to understand BEC is a translation invariant system at given inverse temperature β and chemical potential μ, in the limit that the system size L tends to infinity. In this case, BEC means that

$$\lim_{L \to \infty} \frac{1}{L^3} \underbrace{\sup_{\|f\|=1} \langle a^\dagger(f) a(f) \rangle_{\beta,\mu}}_{\text{largest eigenvalue of } \gamma} > 0.$$

10

For translation invariant systems, γ is also translation invariant and hence has an integral kernel of the form

$$\gamma(x - y) = \frac{1}{L^3} \sum_{p \in \left(\frac{2\pi}{L}\mathbb{Z}\right)^3} \gamma_p\, e^{ip(x-y)}$$

where γ_p denote the eigenvalues of γ. Moreover, for a Hamiltonian of the form

$$H = \sum_{i=1}^{N} p_i^2 + V(x_1, \ldots, x_N)$$

it is also true that γ is positivity improving, meaning that it has a strictly positive integral kernel $\gamma(x - y)$, and hence $\gamma_0 > \gamma_p$ for all $p \neq 0$. Hence the largest eigenvalue is always associated to the constant eigenfunction, and BEC can only occur in the zero momentum mode.

BEC is extremely hard to establish rigorously. In fact, the only known case of an interacting, translation invariant Bose gas where BEC has been proved in the standard thermodynamic limit is the hard-core lattice gas. For completeness, we shall briefly describe it in the following section.

2.2 The Hard-Core Lattice Gas

For a lattice gas, one replaces the continuous configuration space $\mathbb{R}^3$ of a particle by the cubic lattice $\mathbb{Z}^3$. I.e., the one-particle Hilbert space $\mathcal{H}_1$ becomes $\ell^2(\mathbb{Z}^3)$ instead of $L^2(\mathbb{R}^3)$. Other types of lattices are possible, of course, but we restrict our attention to the simple cubic one for simplicity. The appropriate generalization of the Laplacian operator on $\mathbb{R}^3$ is the discrete Laplacian

$$(\Delta\psi)(x) = \sum_{e}(\psi(x + e) - \psi(x)).$$

where the sum is over unit vectors e pointing to the nearest neighbors on the lattice.

We assume that the interaction between particles takes place only on a single site, and that it is sufficiently strong to prevent any two particles from occupying the same site. In this sense, these are hard-core particles. I.e., the interaction energy is zero if all particles occupy different sites, and $+\infty$ otherwise.

Since there is at most one particle at a site x, we can represent the creation and annihilation operators of a particle at a site x as 2×2 matrices

$$a_x^\dagger = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad a_x = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

where the vector $\binom{1}{0}_x$ refers to the state where x is occupied, and $\binom{0}{1}_x$ to the state where x is empty. Also

$$n_x = a_x^\dagger a_x = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

In other words, the appropriate Fock space for this system becomes

$$\mathcal{F} = \bigotimes_{x \in [0,L)^3 \cap \mathbb{Z}^3} \mathbb{C}_x^2$$

and the Hamiltonian (minus the chemical potential times N) equals with

$$H = - \sum_{\langle x,y \rangle} a_x^\dagger a_y - \mu \sum a_x^\dagger a_x.$$

Here, $\langle x, y \rangle$ stands for nearest neighbor pairs on the lattice. The diagonal terms in the discrete Laplacian have been dropped for simplicity, as they can be absorbed into the chemical potential μ.

Note that Fock space is finite dimensional! Moreover, the Hamiltonian looks extremely simple, as it is quadratic in the $a_x^\dagger$ and a_x. However, these are not the usual creation and annihilation operators anymore, as they do not satisfy the canonical commutation relations. In fact,

$$[a_x, a_x^\dagger] = 1 - 2n_x$$

and

$$a_x a_x^\dagger + a_x^\dagger a_x = 1$$

Therefore, at a given site, the system looks like it is fermionic, but for different sites the operators still commute, as appropriate for bosons.

To gain some intuition about the behavior of the system, it is instructive to rewrite the Hamiltonian H in terms of spin operators. Recall that for a spin $1/2$ particle, the three components of the spin are represented by the $1/2$ times the Pauli matrices, i.e., by

$$S^1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S^2 = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad S^3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

If we define, as usual, the spin raising and lowering operators by $S^\pm = S^1 \pm i S^2$, we see that $a^\dagger$ corresponds to S^+, a to S^-, and n to $S^+ S^- = S^3 + 1/2$. Hence, up to an irrelevant constant

$$H = - \sum_{\langle x,y \rangle} S_x^+ S_y^- - \mu \sum_x S_x^3,$$

This is known as the (spin $1/2$) XY model. The chemical potential plays the role of an external magnetic field (in the 3-direction).

The following theorem establishes the existence of BEC in this system at small enough temperature, for a particular value of the chemical potential.

Theorem 1 (Dyson, Lieb, Simon (1978) [4]). *For $\mu = 0$ and T small enough,*

$$\lim_{L \to \infty} \frac{1}{L^3} \left\langle \left(\underbrace{L^{-3/2} \sum_x S_x^+}_{a_{p=0}^\dagger} \right) \left(\underbrace{L^{-3/2} \sum_x S_x^-}_{a_{p=0}} \right) \right\rangle > 0 \qquad (5)$$

We note that $\mu = 0$ corresponds to half-filling, i.e., $\langle N \rangle = L^3/2$, and there is a particle-hole symmetry, implying there are half as many particles as there are lattice sites, on average. The result has only been proved in this special case and it is not known how to extend it to $\mu \neq 0$.

Eq. (5) can be rewritten as

$$\lim_{L \to \infty} \frac{1}{L^6} \sum_{x,y} \left(\langle S_x^+ S_y - \rangle - \underbrace{\langle S_x^+ \rangle \langle S_y^- \rangle}_{=0} \right) > 0$$

since $\langle S_x^+ \rangle = \langle S_y^- \rangle = 0$ by rotation symmetry of H in the 1–2 plane. What this says is that, on average, $\langle S_x^+ S_y - \rangle - \langle S_x^+ \rangle \langle S_y^- \rangle > 0$ even though x and y are macroscopically separated. This property is known as long-range order, and is equivalent to ferromagnetism of the spin system. On average, the value of a spin is zero, but the spins tend to align in the sense that if a spin at some point x points in some directions, all other spins tend to align in the same direction.

The proof of Theorem 1 relies crucially on a special property of the system known as reflection positivity. It extends earlier results by Fröhlich, Simon and Spencer [5] on classical spin systems, where this property was first used to proof the existence of phase transitions. Reflection positivity holds only in the case of particle-hole symmetry, i.e., $\mu = 0$, and hence the proof is restricted to this particular case.

3 Dilute Bose Gases

3.1 The Model

In this section, we return to the description of Bose gases in continuous space. For simplicity, let us consider a system of just one species of particles, with pairwise interaction potential. In practice, the gas will consist of atoms, but we can treat them as point particles as long as the temperature and the density are low enough so that excitations of the atoms are rare. The atoms will behave like bosons if the number of neutrons in their nucleus is even, since then they will have an integer total spin.

The Hamiltonian for such a system is

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \leq i < j \leq N} v\left(|x_i - x_j|\right) \tag{6}$$

where we again choose units such that $\hbar = 1$ and $m = 1/2$. The particles are confined to a cubic box of side length L, and appropriate boundary conditions have to be chosen to make $-\Delta$ a self-adjoint operator. Usually these are Dirichlet boundary conditions (rigid walls) or periodic boundary conditions (torus).

We assume that the interaction is of short range, by which we mean that

$$\int_{|x| \geq R} v(|x|) dx < \infty$$

for some $R \geq 0$. In other words, v should be integrable at infinity. Locally it can be very strong, however. A typical example is a system of hard spheres of diameter R_0, where

$$v(|x|) = \left\{ \begin{array}{ll} +\infty & \text{if } |x| \leq R_0 \\ 0 & \text{if } |x| > R_0 \end{array} \right.$$

The interaction has to be sufficiently repulsive to ensure that the system is a gas for low temperatures and densities. In particular, there should be no bound states of any kind. This is certainly the case if $v(|x|) \geq 0$ for all particle separations $|x|$, which we shall assume henceforth.

So far it has not been possible to prove the existence of BEC (in the usual thermodynamic limit) for such a system, even at low density and for weak interaction v.[1] So our goals have to be more modest here. Let us first investigate the ground state energy of the system, i.e.,

$$E_0(N) = \inf \operatorname{spec} H_N$$

We will be particularly interested in large systems, i.e., in the thermodynamic limit

$$\left. \begin{array}{l} L \to \infty \\ N \to \infty \end{array} \right\} \text{ with } \varrho = \frac{N}{L^3} \text{ fixed}$$

At low density, one might expect that the ground state energy is mainly determined by two-particle collisions, and hence

$$E_0(N) \approx \frac{N(N-1)}{2} E_0(2)$$

That is, the energy should approximately equal the energy of just 2 particles in a large box, multiplied by the total number of pairs of particles. We shall compute $E_0(2)$ in the following.

---

[1]It is possible to prove an upper bound on the critical temperature, however. That is, once can establish the absence of BEC for large enough temperature, see [21].

3.2 The Two-Particle Case

Consider now two particles in a large cubic box of side length L. Ignoring boundary conditions, the two-particle wave function will be of the form $\psi(x_1, x_2) = \phi(x_1 - x_2)$. Hence

$$\frac{\langle \psi | H_2 | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\int \left(2|\nabla \phi(x)|^2 + v(|x|)|\phi(x)|^2 \right) dx}{\int |\phi(x)|^2 dx}$$

since the center-of-mass integration yields L^3 both in the numerator and the denominator. Moreover, since the interaction is short range we can assume that $\phi(x)$ tends to a constant for large $|x|$, and we can take the constant to be 1 without loss of generality. Hence $\int |\phi|^2 = L^3$ to leading order in L.

Definition 1. The *scattering length* a is defined to be

$$a = \frac{1}{8\pi} \inf_\phi \left\{ \int_{\mathbb{R}^3} \left(2|\nabla \phi(x)|^2 + v(|x|)|\phi(x)|^2 \right) dx \; : \; \lim_{|x| \to \infty} \phi(x) = 1 \right\} \tag{7}$$

Note that integrability of $v(|x|)$ at infinity is equivalent to the scattering length a being finite.

With this definition and the preceding arguments, we see that

$$E_0(2) \approx \frac{8\pi a}{L^3}$$

for large L. Hence we expect that

$$E_0(N) \approx \frac{N(N-1)}{2} E_0(2) \approx 4\pi N a \varrho \quad \text{for small } \varrho = N/L^3$$

We will investigate the validity of this formula in the next subsection.

We note that the Euler-Lagrange equation for the minimization problem (7) is

$$-2\Delta \phi(x) + v(|x|)\phi(x) = 0.$$

This is the zero-energy scattering equation. Asymptotically, as $|x| \to \infty$, the solution is of the form

$$\phi(x) \approx 1 - \frac{a}{|x|}$$

with a the scattering length of v. This is easily seen to be an equivalent definition of a, but we shall find the variational characterization (7) to be more useful in the following.

3.3 The Ground State Energy of a Dilute Gas

Consider the ground state energy per particle, $E_0(N)/N$, of the Hamiltonian (6) in the thermodynamic limit

$$e_0(\varrho) = \lim_{N \to \infty} \frac{1}{N} E_0(N) \quad \text{with } L^3 = N/\varrho$$

Based on the discussion above, we expect that

$$e_0(\varrho) \approx 4\pi a \varrho$$

for small density ϱ. This is in fact true.

Theorem 2 (Dyson 1957, Lieb and Yngvason 1998)**.**

$$e_0(\varrho) = 4\pi a \varrho (1 + o(1))$$

with $o(1)$ going to zero as $\varrho \to 0$.

The upper bound was proved by Dyson in 1957 [3] using a variational calculation. He also proved a lower bound, which was 14 times too small, however. The correct lower bound was finally shown in 1998 by Lieb and Yngvason [15].

We remark that the low density limit is very different from the perturbative weak-coupling limit. In fact, at low density the energy is of a particle is very small compared with the the strength of v. The interaction potential is hence very strong but short range. First order perturbation theory, in fact, would predict a ground state energy of the form

$$e_0(\varrho) = \frac{\varrho}{2} \int v(|x|) dx$$

This is strictly bigger than $4\pi a \varrho$, as can be seen from the variational principle (7); $(8\pi)^{-1} \int v$ is the first order Born approximation to the scattering length a.

The proof of Theorem 2 is too lengthy to be given here in full detail, but we shall explain the main ideas. For the upper bound, one can use the variational principle, which says that

$$E_0(N) \leq \frac{\langle \Psi | H_N | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{8}$$

for any Ψ. As a trial function that captures the right two-body physics, one could try a function of the form

$$\Psi(x_1, \ldots, x_N) = \prod_{1 \leq i < j \leq N} \phi(x_i - x_j).$$

The computation of the corresponding energy turns out to be rather tricky, however. One of the reasons for this is that both numerator

16

and denominator on the right side of (8) are exponentially small in the particle number N, and hence cancellations have to be taken into account very carefully. Dyson in fact used a slightly different form of the trial function, and his computation of the upper bound fills several pages.

Before explaining the main ideas in the lower bound by Lieb and Yngvason, let us give some intuition as to why this is a hard problem. It is related to the relevant length scales in the system. Since the energy particle is of the order of $a\varrho$, the associated uncertainty principle length ℓ, obtained by setting this energy equal to ℓ^{-2}, equals

$$\ell \sim \frac{1}{a\varrho}$$

At low density ϱ, this is

$$\ell \sim \frac{1}{\sqrt{a\varrho}} \quad \gg \quad \underbrace{\varrho^{-1/3}}_{\text{mean interparticle separation}} \quad \gg \quad \underbrace{a}_{\text{interaction length}} \quad .$$

Thus, the typical wave functions of a particle is necessarily spread out over a region much bigger than the mean particle distance. The particles hence completely lose their individuality, and behave very quantum (i.e., non-classical) in this sense. Fermions, on the other hand, behave much more classical, since for them $\ell \sim \varrho^{-1/3}$.

The proof of the lower bound on $E_0(N)$ contains two main steps. First, one would like to replace the hard interaction potential v by a soft one, at the expense of kinetic energy. This softer interaction will have a range R, with $a \ll R \ll \varrho^{-1/3}$. Specifically, consider $x_2, \ldots, x_N$ to be fixed for the moment, and assume also that $|x_j - x_k| \geq 2R$ for all $j, k \geq 2$. I.e., assume that the balls $B_R(x_j)$ of radius R centered at x_j are non-overlapping. Then

$$\int \left(|\nabla_1 \psi|^2 + \tfrac{1}{2} \sum_{j \geq 2} v(|x_1 - x_j|)|\psi|^2 \right) dx_1$$

$$\geq \sum_{j \geq 2} \int_{B_R(x_j)} \left(|\nabla_1 \psi|^2 + \tfrac{1}{2} v(|x_1 - x_j|)|\psi|^2 \right) dx_1$$

$$\geq \sum_{j \geq 2} \int U_R(x_1 - x_j)|\psi|^2 dx_1, \tag{9}$$

where

$$U_R(x) = \begin{cases} e(a, R) & |x| \leq R \\ 0 & |x| > R \end{cases}$$

17

and $e(a, R)$ is the lowest eigenvalue of $-\Delta + \frac{1}{2}v$ on B_R, with Neumann boundary conditions. The latter is easily seen to be

$$e(a, R) \approx \frac{4\pi a}{R^3} \quad \text{for } a \ll R \tag{10}$$

as we have already argued in Subsection 3.2.

This is the desired replacing of v by the soft potential U_R. Repeating the above argument for all other particles, we conclude that

$$H_N \geq \sum_{i \neq j} U_R(x_i - x_j)\chi \tag{11}$$

where χ is a characteristic function that makes sure that the balls above do not intersect. I.e., χ removes three-body collisions. In other words, when three particles come close together, we just drop part of the interaction energy. Since $v \geq 0$, this is legitimate for a lower bound.

The soft potential U_R now predicts the correct energy in first order perturbation theory. In fact, for a constant wave function, the expected value of the right side of (11) is approximately equal to $4\pi a N^2/L^3$, with small corrections coming from χ, the region close to the boundary of the box $[0, L]^3$, as well as the fact that (10) is only valid approximately.

To make this perturbative argument rigorous, one keeps a bit of the kinetic energy, and uses

$$H_N \geq -\varepsilon \sum_{i=1}^{N} \Delta_i + (1 - \varepsilon) \sum_{i \neq j} U_R(x_i - x_j)\chi \tag{12}$$

(using positivity of v). First order perturbation theory can easily be seen to be correct if the perturbation is small compared to the gap above the ground state energy of the unperturbed operator. The gap in the spectrum of $-\varepsilon \sum_{i=1}^{N} \Delta_i$ above zero is of the order ε/L^2, which has to be compared with $aN\varrho$. That is, if

$$L^3 a \varrho^2 \ll \frac{\varepsilon}{L^2}, \quad \text{or } L^5 \ll \frac{\varepsilon}{a\varrho^2} \tag{13}$$

then the second term in (12) is truly a small perturbation to the first term and first order perturbation theory can be shown to yield the correct result for the ground state energy.

Condition (13) is certainly not valid in the thermodynamic limit. To get around this problem, one divides the large cube $[0, L]^3$ into many small cubes of side length ℓ, with ℓ satisfying

$$\ell^5 \ll \frac{\varepsilon}{a\varrho^2} = \varrho^{-5/3} \frac{\varepsilon}{a\varrho^{1/3}}$$

For an appropriate choice of ε, the last fraction is big, hence ℓ can be chosen much larger than the mean particle spacing $\varrho^{-1/3}$.

Dividing up space and distributing particles optimally over the cells gives a lower bound to the energy, due to the introduction of additional Neumann boundary conditions on the boundary of the cells. I.e.,

$$E_0(N, L) \geq \min_{\{n_i\}} \sum_i E_0(n_i, \ell)$$

where the minimum is over all distribution of the $N = \sum_i n_i$ particles over the small boxes. Since the interaction is repulsive, it is best to distribute the particles uniformly over the boxes. Hence

$$E_0(N, L) \geq \left(\frac{\ell}{L}\right)^3 E_0(\varrho\ell^3, \ell)$$

For our choice of ℓ, we have $E_0(\varrho\ell^3, \ell) \approx 4\pi a \varrho^2 \ell^3$, as explained above, and hence

$$E_0(N, L) \approx \left(\frac{\ell}{L}\right)^3 4\pi a \varrho^2 \ell^3 = 4\pi a N \varrho$$

This concludes the proof, or at least the sketch of the main ideas.

3.4 Further Rigorous Results

Extending the method presented in the previous subsection, further results about the low-density behavior of quantum gases have been proved. These include

- **Two-Dimensional Bose Gas.** For a Bose gas in two spatial dimensions, it turns out that [16]

$$e_0(\varrho) = \frac{4\pi\varrho}{|\ln(a^2\varrho)|} \quad \text{for } a^2\varrho \ll 1$$

  An interesting feature of this formula is that it does not satisfy $E_0(N) \approx \frac{1}{2}N(N-1)E_0(2)$, as it does in three dimensions. The reason for the appearance of the logarithm is the fact that the solution of the zero energy scattering equation

$$-\Delta\phi(x) + \tfrac{1}{2}v(|x|)\phi(x) = 0$$

  in two dimensions does not converge to a constant as $|x| \to \infty$, but rather goes like $\ln(|x|/a)$, with a the scattering length.

- **Dilute Fermi Gases.** For a (three-dimensional) Fermi gas at low density ϱ, one has [11]

$$e_0(\varrho) = \frac{3}{5}\left(\frac{6\pi^2}{q}\right)^{2/3} \varrho^{2/3} + 4\pi a \left(1 - \frac{1}{q}\right)\varrho + \text{higher order in } \varrho$$

19

Here, q is the number of spin states, i.e., the fermions are considered to have spin $\frac{1}{2}(q-1)$. The first term is just the ground state energy of an ideal Fermi gas. The leading order correction due to the interaction is the same as for bosons, except for the presence of the additional factor $(1-q^{-1})$. Its presence is due to the fact that the interaction between fermions in the same spin states is suppressed, since for them the spatial part of the wave function is antisymmetric and hence vanishes when the particles are at the same location.

A similar result can also be obtained for a two-dimensional Fermi gas [11].

- **Bose Gas at Positive Temperature.** For a dilute Bose gas at positive temperature $T = 1/\beta$, the natural quantity to investigate is the free energy. For an ideal Bose gas, the free energy per unit volume is given by (3), and we shall denote this expression by $f_0(\beta, \varrho)$. For an interaction gas, one has

$$f(\beta, \varrho) = \underbrace{f_0(\beta, \varrho)}_{\text{ideal gas}} + 4\pi a \left(2\varrho^2 - [\varrho - \varrho_c(\beta)]_+^2 \right) + \text{higher order}$$

(14)

and this formula is valid for $a^3\varrho \ll 1$ but $\beta\varrho^{2/3} \gtrsim O(1)$. Here, $\varrho_c(\beta)$ is the critical density for BEC of the ideal gas, given in (2), and $[\,\cdot\,]_+$ denotes the positive part. That is, $[\varrho - \varrho_c(\beta)]_+$ is nothing but the condensate density (of the ideal gas).

Since $\varrho_c(\beta) \to 0$ as $\beta \to \infty$, (14) reproduces the ground state energy formula $4\pi a\varrho^2$ in the zero-temperature limit. Above the critical temperature, i.e., for $\varrho < \varrho_c(\beta)$, the leading order correction is $8\pi a\varrho^2$ instead of $4\pi a\varrho^2$. The additional factor 2 can be understood as arising from the symmetry requirement on the wavefunctions. Because of symmetrization, the probability that 2 bosons are at the same locations is twice as big than on average. This applies only to bosons in different modes, however, since if they are in the same mode, symmetrization has no effect. Hence the subtraction of the square of the condensate density, which does not contribute to the factor 2.

The lower bound on $f(\beta, \varrho)$ of the form (14) was proved in [20], and the corresponding upper bound in [24]. Both articles are rather lengthy and involved, and there are lots of technicalities to turn the above simple heuristics into rigorous bounds. A corresponding result can also be obtained for fermions, as was shown in [19].

For further results and more details, we refer the interested reader to [12].

3.5 The Next Order Term

One of the main open problems concerning the ground state energy of a dilute Bose gas concerns the next order term in an expansion for small ϱ. It is predicted to equal

$$e_0(\varrho) = 4\pi a \varrho \left(1 + \frac{128}{15\sqrt{\pi}} \left(a^3 \varrho \right)^{1/2} + \text{higher order} \right) \qquad (15)$$

This formula was first derived by Lee-Huang-Yang [7], but is essentially already contained in Bogoliubov's famous 1947 paper [1]. The correction term in (15) does not have a simple heuristic explanation, but is a truly quantum-mechanical many-body correlation effect.

The way Bogoliubov arrived at this prediction is the following. The starting point is the Hamiltonian on Fock space. We use plane waves as a basis set, and assume periodic boundary conditions. Then

$$H = \sum_p p^2 a_p^\dagger a_p + \frac{1}{2V} \sum_{p,r,s} \widehat{v}(p) a_{s+p}^\dagger a_{r-p}^\dagger a_r a_s$$

where $V = L^3$ is the volume and

$$\widehat{v}(p) = \int_{\mathbb{R}^3} v(|x|) e^{-ip \cdot x} dx$$

denotes the Fourier transform of v. All sums are over $(\frac{2\pi}{L}\mathbb{Z})^3$. Bogoliubov introduced two approximations, based on the assumption that in the ground state most particles occupy the zero momentum mode. For this reason, one first neglects all terms in H that are higher than quadratic in $a_p^\dagger$ and a_p for $p \neq 0$. Second, one replaces all $a_0^\dagger$ and a_0 by a number $\sqrt{N_0}$, since these operators are expected to have macroscopic values, while there commutator is only one and hence negligible.

The resulting expression for H is the Bogoliubov Hamiltonian

$$H_B = \frac{N^2 - (N - N_0)^2}{2V} \widehat{v}(0)$$
$$+ \sum_{p \neq 0} \left[\left(p^2 + \frac{N_0}{V} \widehat{v}(p) \right) a_p^\dagger a_p + \frac{N_0}{2V} \left(a_p^\dagger a_{-p}^\dagger + a_p a_{-p} \right) \right] \quad (16)$$

This Hamiltonian is now quadratic in creation and annihilation operators, and can be diagonalized easily with the help of a Bogoliubov transformation. The resulting expression for the ground state energy per particles in the thermodynamic limit is

$$4\pi\varrho(a_0 + a_1) + 4\pi\varrho a_0 \frac{128}{15\sqrt{\pi}} \left(a_0^3 \varrho \right)^{1/2} + \text{higher order in } \varrho \qquad (17)$$

where a_0 and a_1 are, respectively, the first and second order Born approximation to the scattering length a. Explicitly,

$$a_0 = \frac{1}{8\pi} \int_{\mathbb{R}^3} v(|x|)dx$$

and

$$a_1 = -\frac{1}{(8\pi)^2} \int_{\mathbb{R}^6} \frac{v(|x|)v(|y|)}{|x-y|} dx\, dy$$

Moreover, in the ground state

$$\left\langle \sum_{p\neq 0} a_p^\dagger a_p \right\rangle \approx N\sqrt{a^3\varrho}$$

hence $(N-N_0)^2 \approx N^2 a^3 \varrho$ is negligible to the order we are interested in.

The expression (17) looks like an expansion of $e_0(\varrho)$ simultaneously in small density and weak coupling. It is hence reasonable to expect the validity of (15) without the weak coupling assumption. The proof of this fact is still an open problem, however. For smooth interaction potentials, an upper bound of the correct form was recently proved in [23]. There was also some recent progress in [6] concerning the lower bound, where it was shown that Bogoliubov's approximation is correct, as far as the ground state energy is concerned, if one is allowed to rescale the interaction potential v with ϱ is a suitable way.

We remark that the Bogoliubov Hamiltonian (16) not only gives a prediction about the ground state energy, but also about the excitation spectrum. Diagonalizing H_B leads to an excitation spectrum of the form

$$\sqrt{p^4 + 2p^2\varrho\hat{v}(p)}$$

which is linear for small momentum p. The non-zero slope at $p = 0$ is in fact extremely important physically and has many interesting consequences, concerning superfluidity, for instance. It is also confirmed experimentally. A rigorous proof that the Bogoliubov approximation indeed predicts the correct low energy excitation spectrum is still lacking, however.

4 Dilute Bose Gases in Traps

4.1 The Gross-Pitaevskii Energy Functional

Actual experiments on cold atomic gases concern inhomogeneous systems, since the particles are confined to a trap with soft walls. Let us extend the analysis of the previous sections to see what happens in the inhomogeneous case.

Let $V(x)$ denote the trap potential, and $\varrho(x) = |\phi(x)|^2$ the particle density at a point $x \in \mathbb{R}^3$. If V varies slowly, we can use a local density approximation and assume the validity of the formula $4\pi a \varrho^2$ for the energy density of a dilute gas even locally. In this way, we arrive at the expression

$$\mathcal{E}^{\mathrm{GP}}(\phi) = \int_{\mathbb{R}^3} |\nabla \phi(x)|^2 dx + \int_{\mathbb{R}^3} V(x)|\phi(x)|^2 dx + 4\pi a \int_{\mathbb{R}^3} |\phi(x)|^4 dx$$
(18)

which is known as the *Gross-Pitaevskii (GP) functional.* The last two terms are simply the trap energy and the interaction energy density of a dilute gas in the local density approximation. The first gradient term is added to ensure accuracy even at weak or zero interaction. In fact, for an ideal, $a = 0$ and hence (18) is certainly the correct description of the energy of the system in this case.

Minimizing (18) under the normalization constraint $\int |\phi(x)|^2 dx = N$ leads to the GP energy

$$E^{\mathrm{GP}}(N, a) = \min \left\{ \mathcal{E}^{\mathrm{GP}}(\phi) \ : \ \int |\phi(x)|^2 dx = N \right\} \qquad (19)$$

Using standard techniques of functional analysis (see Appendix A of [13]) one can show that there is a minimizer for this problem, which is moreover unique up to a constant phase factor. This holds under suitable assumptions on the trap potential $V(x)$, e.g., if V is locally bounded and tends to infinity as $|x| \to \infty$. The minimizer satisfies the corresponding Euler-Lagrange equation

$$-\Delta \phi + V\phi + 8\pi a |\phi|^2 \phi = \mu \phi,$$

which is a nonlinear Schrödinger equation called the GP equation. The chemical potential μ equals $\partial E^{\mathrm{GP}}/\partial N$ and is the appropriate Lagrange parameter to take the normalization condition on ϕ into account.

Based on the discussion above, one would expect that

$$E_0 \approx E^{\mathrm{GP}}$$

and also

$$\varrho_0(x) \approx |\phi^{\mathrm{GP}}(x)|^2$$

where E_0 and ϱ_0 are the ground state energy and corresponding particle density, respectively. This approximation should be valid if V varies slowly and the gas is sufficiently dilute.

Notice that the GP energy $E^{\mathrm{GP}}(N, a)$ and the corresponding minimizer $\phi_{N,a}^{\mathrm{GP}}$ satisfy the simple scaling relations

$$E^{\mathrm{GP}}(N, a) = N E^{\mathrm{GP}}(1, Na) \quad \text{and} \quad \phi_{N,a}^{\mathrm{GP}}(x) = \sqrt{N} \phi_{1,Na}^{\mathrm{GP}}(x)$$

i.e., Na is the only relevant parameter for the GP theory. In particular, for the purpose of deriving the GP theory from the many-body problem, it makes sense to take N large while Na is fixed. The latter quantity should really be thought of as Na/L, where L is the length scale of the trap V. Hence $a/L \sim N^{-1}$, i.e., V varies indeed much slower that the interaction potential. We shall choose units to make $L = 1$, which simplifies the notation.

Since V is now fixed, we have to rescale the interaction potential v. The appropriate way to do this is to write

$$v_a(|x|) = \frac{1}{a^2} w(|x|/a)$$

for some fixed w. It is then easy to see that v_a has scattering length a if w has scattering length 1. The appropriate many-body Hamiltonian under consideration is thus

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

In this way, a enters as a parameter which can now be varied with N. In particular, the ground state energy $E_0 = \inf \operatorname{spec} H_N$ is now a function of N and a. We shall therefore write $E_0(N, a)$, but suppress the dependence on N and a of the ground state density $\varrho_0(x)$ in the notation for simplicity.

Theorem 3 (Lieb-S-Yngvason '00 [13]).

$$\lim_{N\to\infty} \frac{E_0(N, g/N)}{N} = E^{\mathrm{GP}}(1, g) \quad \text{for any } g \geq 0$$

In the same limit

$$\lim_{N\to\infty} \frac{1}{N} \varrho_0(x) = \left| \phi_{1,g}^{\mathrm{GP}}(x) \right|^2$$

Note that in the limit under consideration $a^3 \bar{\varrho} \sim N^{-2}$, where $\bar{\varrho} \sim N$ denotes the average density. In particular, the gas is very dilute if $g = Na$ is fixed. The result of Theorem 3 is actually uniform in g as long $a^3 \bar{\varrho} \to 0$ as $N \to \infty$. I.e., g is allowed to go to ∞ with N at a suitable rate, as long as the gas stays dilute.

The proof of Theorem 3 is similar to the homogeneous case, and uses the same ideas in the lower bound. In particular, space is divided up into small boxes and the particles are then distributed optimally over these boxes. In the inhomogeneous case consider here, the distribution will be non-uniform, of course.

4.2 BEC of Dilute Trapped Gases

So far the discussion has focused on the ground state energy and the corresponding particle density. But what about BEC? As discussed in Section 2, BEC is a property of the reduced one-particle density matrix of the system. Specifically, if Ψ_0 is the ground state of H_N, then the one-particle density matrix γ is the operator on $L^2(\mathbb{R}^3)$ with integral kernel

$$\gamma_0(x, x') = N \int \Psi_0(x, x_2, \ldots, x_N) \Psi_0(x', x_2, \ldots, x_N)^* dx_2 \cdots dx_N$$

Recall that γ is a positive trace-class operator, with $\operatorname{Tr} \gamma = N$.

Theorem 4 (Lieb-S '02 [9]). *In the same limit as in Theorem 3*

$$\lim_{N \to \infty} \frac{1}{N} \gamma_0 = \left| \phi_{1,g}^{\mathrm{GP}} \right\rangle \left\langle \phi_{1,g}^{\mathrm{GP}} \right|$$

What the theorem says is that there is complete BEC, in the sense that the largest eigenvalue of γ_0, divided by N, is not only non-zero but actually equal to one in the dilute limit considered. I.e., the one-particle density matrix becomes a rank-one projection in the limit, just like for a non-interacting gas. The condensate wave function $\phi_{1,g}^{\mathrm{GP}}$ still depends on the interacting strength via g, however, and might have very little overlap with the non-interacting state at $g = 0$ if g is large.

Theorem 4 represents the only known case of a continuous system with genuine interactions where BEC has been proved. The proof is so far restricted to zero temperature and to the very dilute limit where $a^3 \bar{\varrho} \sim N^{-2}$ as $N \to \infty$.

Before discussing the proof of Theorem 4, we shall first generalize the setting in a non-trivial way by allowing the system to rotate about a fixed axis. Theorem 4 can thus be considered as a special case of a more general result to be discussed next.

4.3 Rotating Bose Gases

An interesting property of dilute cold Bose gases is their response to rotation. In fact, rotating Bose-Einstein condensates are nowadays routinely created in the lab, by stirring the system much like coffee with a spoon.

Even though the system under consideration is now rotating, we can still think of it as being at equilibrium if we go to the rotating frame of reference. Just like in classical mechanics, the only effect of this transformation on the Hamiltonian is to add a term proportional to the total angular momentum. More precisely,

$$H_N \longrightarrow H_N - \Omega \cdot L$$

where $\Omega \in \mathbb{R}^3$ denotes the angular velocity (having an axis and a magnitude) and $L = \sum_{i=1}^{N} L_i$ denotes the total angular momentum of the system.

In the experiments on rotating gases, one observes the appearance of quantized vortices, related to the superfluid properties of the system. This is schematically sketched in Figure 3.
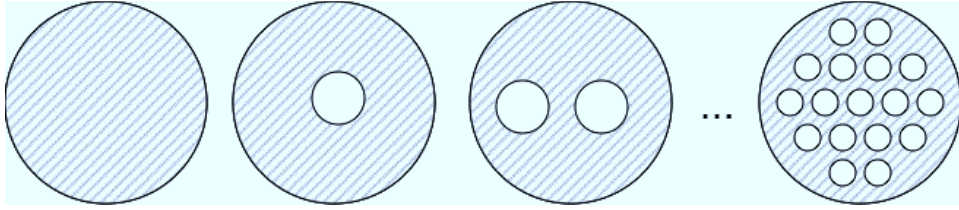

Figure 3: Quantized vortices in a rotating Bose condensate, showing up as holes in the density. More and more vortices appear as the angular velocity is increased. For actual snapshots of experiments, see `http://jila.colorado.edu/bec/hi_res_pic_album_macromedia` or `http://www.bec.nist.gov/gallery.html`.

The quantized vortices can also be seen by minimizing the appropriate GP functional, which now reads

$$\mathcal{E}^{\mathrm{GP}}(\phi) = \langle \phi \,|-\Delta + V(x) - \Omega \cdot L|\, \phi \rangle + 4\pi a \int_{\mathbb{R}^3} |\phi(x)|^4 dx$$

with $L = -ix \wedge \nabla$, as usual. In order for the confining force to overcome the centrifugal force, we have to assume that

$$V(x) - \frac{1}{4}|\Omega \wedge x|^2 \tag{20}$$

is bounded below and goes to infinity at infinity. Under this condition, one can still prove the existence of a minimizer of the GP functional. In general it will not be unique anymore, however. This non-uniqueness is related to spontaneous symmetry breaking. In fact, if V is rotation symmetric about the Ω axis, i.e, $[V, \Omega \cdot L] = 0$, then $\mathcal{E}^{\mathrm{GP}}$ is invariant under rotations about this axis. In general, a minimizer ϕ^{GP} will not have this symmetry, however, due to the appearance of quantized vortices. If there are more than one, these obviously can not be arranged in a symmetric way. I.e, in general we expect a whole continuum of minimizers in the case the GP functional is rotation symmetric.

The N-body Hamiltonian under consideration now is

$$H_N = \sum_{i=1}^{N} (-\Delta_i + V(x_i) - \Omega \cdot L_i) + \sum_{i<j} v_a(|x_i - x_j|).$$

It ground state energy will be denotes by $E_0(N, a, \Omega)$.

Theorem 5 (Lieb-S '06 [10]). *For any $g \geq 0$ and $\Omega \in \mathbb{R}^3$ (subject to the constraint that (20) in bounded from below and goes to infinity at infinity)*

$$\lim_{N \to \infty} \frac{E_0(N, g/N, \Omega)}{N} = E^{\mathrm{GP}}(1, g, \Omega)$$

Moreover, up to a subsequence, the one-particle density matrix of a ground state (or any approximate ground state, in fact) satisfies

$$\lim_{N \to \infty} \frac{1}{N} \gamma = \int d\mu \, |\phi^{\mathrm{GP}}\rangle \langle \phi^{\mathrm{GP}}| \tag{21}$$

where $d\mu$ is a probability measure on the set of minimizers of $\mathcal{E}^{\mathrm{GP}}$.

By an approximate minimizer we mean a state that has the same energy as the ground state energy, to leading order. In other words, a state with energy equal to

$$\lim \frac{1}{N} \langle H_N \rangle = E^{\mathrm{GP}}(1, g, \Omega)$$

in the limit $N \to \infty$, $Na \to g$.

Eq. (21) is the natural generalization of complete BEC in the case of non-uniqueness of GP minimizers. Because of the linearity of quantum mechanics, the best one can hope for is a convex combination of completely condensed states. In fact, (21) can also be seen as establishing the spontaneous symmetry breaking mentioned earlier. Under an infinitesimal perturbation, the GP functional will generically have a unique minimizer, and Theorem 5 in this case implies that there is then complete BEC in the usual sense.

We note the the bosonic symmetry requirement on the N-particle wave functions is crucial for Theorem 5 to hold. In contrast, for the discussion of the ground state of non-rotating systems, Bose symmetry does not have to be enforced explicitly, it comes out automatically as the ground state of an operator of the form $-\Delta + W(x)$ is always unique and positive and hence can only be permutation symmetric. For rotating systems, this is generally not the case, and Bose symmetry can not be ignored.

4.4 Main Ideas in the Proof

We split the proof of Theorem 5 into three parts.

Step 1. The first step is again to try to replace the hard interaction potential $v_a(|x|)$ by a softer one, $U_R(|x|)$, at the expense of some kinetic energy. We must not use up all the kinetic energy as we did in the homogeneous case, however, since we still need to obtain the gradient

term in the GP functional. The key idea is to split the kinetic energy into a high momentum and a low momentum part. Only the high momentum part $|p| \geq p_c$ will be needed to achieve the replacement $v_a \to U_R$, while the low momentum part $|p| \leq p_c$ will kept as it is needed in the GP functional. We will, in fact choose

$$1 \ll p_c \ll \frac{1}{R} \tag{22}$$

The first condition implies that only momentum irrelevant for the GP functional are being used, while the second makes sure that all momentum relevant on the length scale of U_R are actually employed. The crucial Lemma that improves (9) is the following. Its proof is in [11].

Lemma 1. *Let $\chi_{B_R(0)}$ denote the characteristic function of the ball of radius R centered at the origin. For any $0 < \varepsilon < 1$,*

$$-\nabla \cdot \xi(p)\chi_{B_R(0)}(x)\xi(p)\nabla + \frac{1}{2}v(|x|) \geq (1 - \varepsilon)U_R(|x|) - \frac{1}{\varepsilon}w_R(x) \tag{23}$$

where

$$w_R(x) = \frac{2a}{\pi^2}f_R(x)\int_{\mathbb{R}^3} f_R(y)dy$$

and $f_R(x) = \sup_{|y| \leq R}|h(x - y) - h(x)|$, $\widehat{h}(p) = 1 - \xi(p)$.

The function ξ is chosen to be a smooth characteristic function of the set $\{|p| \geq p_c\}$. Hence the first term in (23) is a version of the Laplacian that has been restricted to high momentum and localized to a Ball of radius R (centered at the origin). The price one has to pay for the cut-off ξ is the error term w_R, which is supported also outside the ball but can be made to decay very fast by choose ξ smooth. For our choice of p_c in (22), it will be negligible compared to U_R.

Lemma 1 implies the operator lower bound

$$H_N \geq \sum_{i=1}^{N} \left(-\Delta_i(1 - \xi(p_i)^2) + V(x) - \Omega \cdot L_i\right)$$
$$+ \sum_{i \neq j} \left((1 - \varepsilon)U_R(|x_i - x_j|) - \frac{1}{\varepsilon}w_R(|x_i - x_j|)\right)\chi \tag{24}$$

where χ is again a characteristic function that excludes three- and more particle collisions.

Step 2. In order to proceed, we want to get rid of both the w_R term and the characteristic function χ in (24). For this purpose, we need some *a priori* bounds that tell us that the expected values of w_R and $1 - \chi$ in the ground state of H_N are not too big. For this purpose, we obtained some rough bounds on the three-particle density

of a ground state of H_N, using path integrals. These bounds are of the form
$$\langle f(x_1, x_2, x_3)\rangle \leq \Lambda(\alpha, f)\, e^{\alpha(E_0(N)-E_0(N-3))}$$

where $\langle\,\cdot\,\rangle$ denotes expectation in the zero-temperature state, f is an arbitrary positive bounded function, $\alpha > 0$ is arbitrary and $\Lambda(\alpha, f)$ denotes the largest eigenvalue of the operator
$$\sqrt{f}\, e^{-\alpha(-\Delta_1-\Delta_2-\Delta_3+V(x_1)+V(x_2)+V(x_3))}\sqrt{f}$$

on $L^2(\mathbb{R}^9)$. This bound is certainly not optimal, but suffices to show that the terms in question due not contribute to the ground state energy to the order we are interested. I.e., we conclude that
$$\inf\mathrm{spec}\, H_N \geq \inf\mathrm{spec}\, \widetilde{H}_N - \delta N$$

where $\delta \to 0$ in the limit considered. Moreover,

$$\widetilde{H}_N = \sum_{i=1}^{N}\left(-\Delta_i(1-\xi(p_i)^2) + V(x) - \Omega\cdot L_i\right) + \sum_{i\neq j}U_R(|x_i - x_j|) \quad (25)$$

That is, we have managed to genuinely replace the hard interaction potential v_a by the soft one U_R, at the expense of the high-momentum part of the kinetic energy, as well as a minor shift in the ground state energy.

Step 3. Let us denote the one-particle part of the Hamiltonian $\widetilde{H}_N$ by h for simplicity, i.e.,
$$h = -\Delta(1-\xi(p)^2) + V(x) - \Omega\cdot L$$

In second quantized form, using as a basis the eigenstates of h, we have

$$\widetilde{H} = \sum_i\langle\varphi_i|h|\varphi_i\rangle a_i^\dagger a_i + \sum_{ijkl}\langle\varphi_i\otimes\varphi_j|U_R|\varphi_k\otimes\varphi_l\rangle a_i^\dagger a_j^\dagger a_k a_l \quad (26)$$

Notice that if we ignore all commutators between the $a_i^\dagger$ and a_i and treat them as numbers, z_i^* and z_i, respectively, (26) becomes

$$\langle\Phi|h|\Phi\rangle + \int_{\mathbb{R}^6}|\Phi(x)|^2 U_R(|x-y|)|\Phi(y)|^2\, dx\, dy$$

with
$$\Phi(x) = \sum_i z_i\varphi_i(x)$$

This is essentially the GP functional, except for the cutoff in the kinetic energy, which is irrelevant for $p_c \gg 1$, and the fact that the interaction

is U_R instead of $4\pi a\delta$. Since $R \ll 1$, however, and $\int U_R = 4\pi a$, U_R is an approximate δ function with the correct coefficient.

In other words, the GP functional emerges from the many-body Hamiltonian on Fock space in a classical limit, replacing all the creation and annihilation operators by complex numbers. In this sense, GP theory is a classical field approximation to the quantum field theory defined by $\widetilde{H}$. Note that this is only true for the low momentum part, however. It is important that we have already completed Step 1 above to replace the true interaction potential v_a by U_R. If we had not done so, the classical approximation would also look like a GP functional, but with the wrong coefficient $\frac{1}{2}\int v$ instead of $4\pi a$ in front of the quartic term.

What remains to be done is to investigate the validity of the replacement of the creation and annihilation operators by numbers. This can be conveniently done using coherent states. We shall describe what these are in the next subsection, and complete the sketch of the proof of Theorem 5 there.

4.5   Coherent States

With $|0\rangle$ denoting the Fock space vacuum, and $z \in \mathbb{C}$, consider the state of Fock space

$$|z\rangle = e^{za^{\dagger} - z^* a}|0\rangle$$

where a and $a^{\dagger}$ are the annihilation and creation operators for one particular mode. Since the exponent is anti-hermitian, $|z\rangle$ is a vector of length one. Because of $[a, a^{\dagger}] = 1$, one can rewrite it also as

$$|z\rangle = e^{-|z|^2/2} e^{za^{\dagger}}|0\rangle$$

This state is a superposition of all states with different particle number in the mode under consideration. As z varies over the complex plane $\mathbb{C}$, the states $|z\rangle$ span the whole Fock space associated with the mode a. In fact, one can easily check the completeness relation

$$\int_{\mathbb{C}} \frac{dz}{\pi}|z\rangle\langle z| = 1$$

where dz stands for the standard Lebesgue measure $dx\,dy$, $z = x + iy$. States with different value of z are of course not orthogonal. One can also check that

$$a|z\rangle = z|z\rangle$$

i.e., $|z\rangle$ is an eigenstate of a with eigenvalue z.

For a general operator given in terms of a and $a^{\dagger}$ (typically a polynomial), define its *lower symbol* $h_l(z)$ by

$$h_l(z) = \langle z|h|z\rangle$$

Note that if h is normal ordered, i.e, all creation operators appear to the left of all annihilation operators, then $h_l(z)$ is obtained from h simply by replacing all a's by z and all $a^\dagger$'s by z^*. Many operators (in particular, all polynomials) also have *upper symbols*, which are functions $h_u(z)$ such that

$$h = \int_{\mathbb{C}} \frac{dz}{\pi} h_u(z) |z\rangle\langle z|$$

In fact, $h_u(z)$ is obtained by replacing a by z and $a^\dagger$ by z^* in the anti-normal ordered form of h.

Examples:

h	$h_l(z)$	$h_u(z)$
a	z	z
$a^\dagger$	z^*	z^*
$a^\dagger a$	$|z|^2$	$|z|^2 - 1$

In general, one can show that $h_l(z)$ and $h_u(z)$ are related by

$$h_u(z) = e^{-\partial_{z^*}\partial_z} h_l(z)$$

(as long as the right side exists).

Note that for self-adjoint h

$$\inf_z h_u(z) \leq \inf \operatorname{spec} h \leq \inf_z h_l(z)$$

The same is true for partition functions, namely the Berezin-Lieb inequalities

$$\int_{\mathbb{C}} \frac{dz}{\pi} e^{-h_l(z)} \leq \operatorname{Tr} e^{-h} \leq \int_{\mathbb{C}} \frac{dz}{\pi} e^{-h_u(z)}$$

hold. These inequalities are, in fact, the origin of the terminology "upper" and "lower" symbols; Upper symbols give upper bounds to the partition function, while lower symbols give lower bounds.

Effectively, coherent states replace a quantum problem by a classical problem with phase space $\mathbb{C}$, replacing creation and annihilation operators by numbers. Note that the difference in the upper and lower bounds comes from the difference in the upper and lower symbols, in particular the factor -1 for the quadratic operator $a^\dagger a$ in the example above.

Coherent states can be used for many modes at the same time, simply using tensor products. One can not use them for *all* modes, however. Even for the number operator, the upper and lower symbols differ by a constant which is the number of modes, and we want to avoid infinities.

31

Let us split the Fock space into two parts,

$$\mathcal{F} = \mathcal{F}_< \otimes \mathcal{F}_>$$

corresponding to the splitting of the one-particle Hilbert space $\mathcal{H}_1$ into $\mathcal{H}_< \oplus \mathcal{H}_>$, where $\mathcal{H}_<$ is a finite dimensional space spanned by the modes $\varphi_1, \ldots, \varphi_J$. Here, $J \geq 0$ is some large finite number to be determined later. On $\mathcal{F}_<$, we can use coherent states for all the modes. In particular, for $\widetilde{H}$, our Hamiltonian under consideration, we can write

$$\widetilde{H} = \int_{\mathbb{C}^J} \prod_{j=1}^{J} \frac{dz_j}{\pi} \, |z_1 \otimes \cdots \otimes z_J\rangle\langle z_1 \otimes \cdots \otimes z_J| \otimes K(z_1, \ldots, z_J)$$

where the upper symbol $K(z_1, \ldots, z_J)$ is now an operator on $\mathcal{F}_>$, the Fock space for the large modes. The key point of this decomposition is that that

$$\inf \operatorname{spec} \widetilde{H} \geq \inf_{z_1, \ldots, z_J} \inf \operatorname{spec} K(z_1, \ldots, z_J)$$

One can show that, for $J \gg 1$ appropriately chosen

$$K(z_1, \ldots, z_J) = \mathcal{E}^{\mathrm{GP}}(\Phi) + \text{error terms}$$

where

$$\Phi(x) = \sum_{j=1}^{J} z_j \varphi_j(x)$$

The error terms are still operators on $\mathcal{F}_>$, but they are small (at least in expectation) for an appropriate choice of the interaction range R. For these estimates, it is important that $R \gg a \sim N^{-1}$, hence the necessity of Step 1. If fact, the larger R the better the control of the error terms, but we can still get away with some $R \ll N^{-1/3}$, as required.

This completes the sketch of the proof of the lower bound to the ground state energy in Theorem 5. For the details, we refer to [10]. An appropriate upper bound can be derived using the variational principle [18].

For the proof of BEC, one can proceed as above, but adding to the one-particle Hamiltonian some perturbation S. The proof goes through essentially without change, since the precise form of h has never been used. The result is the validity of the GP theory for the ground state energy, even with h replaced by $h + S$. One can now use standard convexity theory, differentiation with respect to S. The key point is this: If concave functions $f_n(x)$ converge pointwise to a function f,

then the right and left derivatives f'_+ and f'_- (which always exist for concave functions) satisfy

$$f'_+(x) \leq \liminf_{n \to \infty} f'_{n,+}(x) \leq \limsup_{n \to \infty} f'_{n,-}(x) \leq f'_-(x) \qquad (27)$$

In particular, if f is differentiable at a point x, then there is equality everywhere in (27).

The left and right derivatives of

$$\lambda \mapsto \inf_{\phi} \left(\mathcal{E}^{\mathrm{GP}}(\phi) + \lambda \langle \phi | S | \phi \rangle \right)$$

at $\lambda = 0$ are both of the form $\langle \phi^{\mathrm{GP}} | S | \phi^{\mathrm{GP}} \rangle$, with ϕ^{GP} a GP minimizer (in the case $\lambda = 0$). They need not be the same, however. We thus conclude that

$$\min_{\phi^{\mathrm{GP}}} \langle \phi^{\mathrm{GP}} | S | \phi^{\mathrm{GP}} \rangle \leq \lim_{N \to \infty} \frac{1}{N} \mathrm{Tr}\, S\gamma \leq \max_{\phi^{\mathrm{GP}}} \langle \phi^{\mathrm{GP}} | S | \phi^{\mathrm{GP}} \rangle \qquad (28)$$

for the one-particle density matrix γ of a ground state of H_N, where the maximum and minimum, respectively, is over all minimizers of the GP functional. Since (28) is valid for all (hermitian, bounded) S, the statement about BEC follows now quite easily. For simplicity, just consider the case of a unique GP minimizer, in which case there is equality in (28). It is easy to see that this implies $\lim_{N \to \infty} N^{-1}\gamma = |\phi^{\mathrm{GP}}\rangle \langle \phi^{\mathrm{GP}}|$. The more general case is discussed in detail in [10].

4.6 Rapidly Rotating Bose Gases

Consider now the special case of a harmonic trap potential

$$V(x) = \frac{1}{4}|x|^2$$

This is of particular relevance for the experimental situation, where the trap potential is typically close to being harmonic. The one-particle part of the Hamiltonian can then be written as

$$h = -\Delta + V(x) - \Omega \cdot L = \left(-i\nabla - \tfrac{1}{2}\Omega \wedge x \right)^2 + \tfrac{1}{4}\left(|x|^2 - |\Omega \wedge x|^2 \right)$$

The first part on the right side is the same as the kinetic energy of a particle in a homogeneous magnetic field Ω and, in particular, is translation invariant (up to a gauge transformation). It follows that h is bounded from below only for $|\Omega| \leq 1$. The angular velocity has to be less than one, otherwise the trapping force is not strong enough to compensate the centrifugal force and the system flies apart.

What happens to a dilute Bose gas as $|\Omega|$ approaches 1? For $e = \Omega/|\Omega|$ the rotation axis, let us rewrite h as

$$h = \underbrace{\left(-i\nabla - \tfrac{1}{2}e \wedge x \right)^2 + \tfrac{1}{4}|e \cdot x|^2}_{k} + (e - \Omega) \cdot L$$

33

For Ω close to e, the last term can be considered as a perturbation of the rest, which we denote by k. The spectrum of k equals $\{3/2, 5/2, 7/2, \dots\}$, and each energy level is infinitely degenerate. These energy levels are in fact just the Landau levels for a particle in a homogeneous magnetic field (for the motion perpendicular to Ω), combined with a simple harmonic oscillator in the Ω direction.

For $|e - \Omega| \ll 1$, we can thus restrict the one-particle Hilbert space to the lowest Landau level (LLL) when investigating the low energy behavior of the system. This LLL consists of functions of the form

$$f(z)e^{-|x|^2/4}$$

where we use a complex variable z for the coordinates perpendicular to Ω. In particular, $|x|^2 = |z|^2 + |e \cdot x|^2$. Moreover, the function f has to be analytic, i.e., it is an entire function of z. The only freedom lies in the choice of f, in fact, the Gaussian factor is fixed. In particular, the motion in the Ω direction is frozen into the ground state of the harmonic oscillator. Because of that, it is convenient to think of the Hilbert space as the space of analytic functions f only, and absorb the Gaussian into the measure. The resulting space is known as the Bargmann space

$$\mathcal{B} = \left\{ f : \mathbb{C} \to \mathbb{C} \text{ analytic}, \ \int_{\mathbb{C}} |f(z)|^2 e^{-|z|^2/2} dz < \infty \right\}$$

On the space $\mathcal{B}$, the angular momentum $e \cdot L$ simply acts as

$$L = z \frac{\partial}{\partial z}$$

In particular, its eigenstates are z^n, $n = 0, 1, 2, \dots$. These states form an orthonormal bases of $\mathcal{B}$. In particular, note that $L \geq 0$ on $\mathcal{B}$.

Having identified the relevant one-particle Hilbert space for the low energy physics of a rapidly rotating Bose gas, what should the relevant many-body Hamiltonian look like? The only term left from the one-particle part of H_N is $(e - \Omega) \cdot L$. If we assume that the interaction is short range, i.e, $a \ll 1$ (where 1 is the relevant "magnetic length" in our units), in can be approximated by δ-function in the LLL. I.e., we introduce as a many-body Hamiltonian on $\mathcal{B}^{\otimes N}$

$$H_N^{\text{LLL}} = \omega \sum_{i=1}^{N} z_i \frac{\partial}{\partial z_i} + 8\pi a \sum_{1 \leq i < j \leq N} \delta_{ij} \tag{29}$$

where $\omega > 0$ is short for $1 - |\Omega|$ and δ_{ij} is obtained from projecting $\delta(x_i - x_j)$ onto the LLL level. Explicitly, we have

$$\left(\delta_{12} f \right)(z_1, z_2) = (2\pi)^{-3/2} f\left(\tfrac{1}{2}(z_1 + z_2), \tfrac{1}{2}(z_1 + z_2) \right)$$

That is, δ_{12} symmetrizes the arguments z_1 and z_2. In particular, it takes analytic functions into analytic functions. Except for the unimportant prefactor $(2\pi)^{-3/2}$, δ_{12} is, in fact, a projection, projecting onto relative angular momentum zero. The factor $8\pi a$ in front of the interaction term in (29) is chosen as to reproduce the correct expression for the ground state energy of a homogeneous system.

The introduction of the effective many-body Hamiltonian H_N^{LLL} in the lowest Landau level raises interesting questions. First of all, can one rigorously justify the approximations leading to H_N^{LLL}? In other words, can it be rigorously derived from the full many-body problem, defined by H_N on the entire Hilbert space? This was indeed achieved in [8], where it was shown that for small ω and small a, the low energy spectrum and corresponding eigenstates of H_N are indeed well approximated by the corresponding ones of H_N^{LLL}, and converge to these in the limit $\omega \to 0$, $a \to 0$ with a/ω fixed. Note that H_N^{LLL} can *not* be obtained by simply projecting H_N onto the LLL, as this would not reproduce the correct prefactor $8\pi a$ in front of the interaction. It is important to first integrate out the high energy degrees of freedom, associated with length scales much smaller than 1, as we have done several times earlier. The projection onto the LLL is only a good approximation for length scales of order one and larger.

Having rigorously derived H_N^{LLL} from the full many-body problem, what have we learned? It still remains to investigate the relevant properties of this effective model, in particular its spectrum and corresponding eigenstates. Relatively little is known about these questions, however, despite the apparent simplicity of the model. Interesting behavior reminiscent of the fractional quantum Hall effect in fermionic systems is expected.

Note that H_N^{LLL} is the sum of two terms

$$H_N^{\mathrm{LLL}} = \omega \underbrace{\sum_{i=1}^{N} z_i \frac{\partial}{\partial z_i}}_{L_N} + 8\pi a \underbrace{\sum_{1 \le i < j \le N} \delta_{ij}}_{\Delta_N} \tag{30}$$

that commute with each other, i.e., $[L_N, \Delta_N] = 0$. It therefore makes sense to look at their joint spectrum. Of particular relevance is the so-called "yrast curve", which is the lowest energy of Δ_N is a given sector of angular momentum. That is,

$$\Delta_N(L) = \inf \mathrm{spec}\, \Delta_N \upharpoonright_{L_N = L}$$

It is known explicitly for small and large L. In fact, the known values of $\Delta_N(L)$ are

$$\Delta_N(L) = \frac{1}{2(2\pi)^{3/2}} \times \begin{cases} N(N-1) & L \in \{0, 1\} \\ N(N-1-\frac{1}{2}L) & 2 \le L \le N \\ 0 & L \ge N(N-1) \end{cases}$$

The minimizer for $L = N(N - 1)$ is in fact the bosonic analogue for the Laughlin state

$$\prod_{i<j}(z_i - z_j)^2$$

for which obviously the interaction energy is zero. Note the exponent 2, which has to be even since we are dealing with bosons.
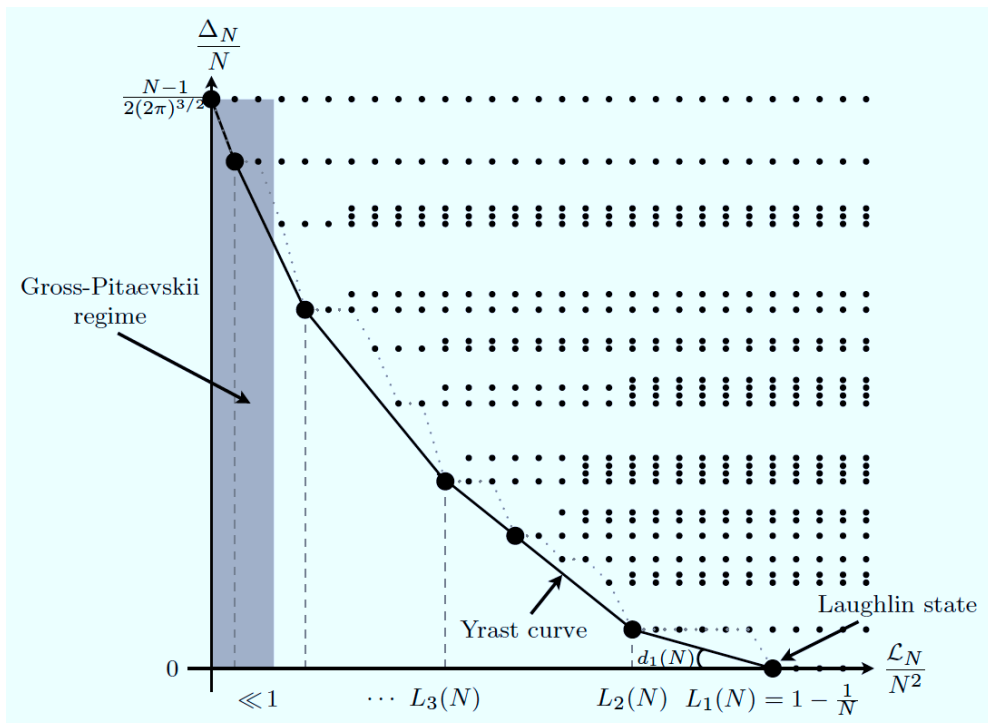

Figure 4: Sketch of the joint spectrum of L_N and Δ_N. The GP approximation is valid in the shaded region on the left. The small dots show the yrast curve, in black is its convex hull. The bold dots on the convex hull are, in fact, the possible ground states of H_N^{LLL} as one varies ω/a.

A sketch of the joint spectrum of L_N and Δ_N is given in Figure 4. The interesting part concerns angular momenta of order N^2, in which case Δ_N is of order N. For $L \ll N^2$, one can show that the GP approximation becomes exact. I.e., for large N and $L \ll N^2$, the convex hull of $\Delta_N(L)$ is given by

$$\inf_{\phi \in B}\left\{\int_{\mathbb{C}} |\phi(z)|^4 e^{-|z|^2} dz \;:\; \|\phi\|^2 = N, \langle\phi|L|\phi\rangle = L\right\}$$

This was proved in [14] using coherent states. The condition $L \ll N^2$ corresponds to the case when the number of particles is much

larger than the number of vortices. Once these two numbers becomes comparable, the GP approximation breaks down and interesting new physics with highly correlated many-body states is expected to occur.

No rigorous bounds on $\Delta_N(L)$ are available for $L \sim N^2$ (but $L < N(N-1)$, of course). In fact, even to prove the existence of the limit

$$\lim_{N \to \infty} \frac{\Delta_N(\ell N^2)}{N}$$

is an open problem. Besides $\Delta_N(L)$, one would also like to understand the existence or non-existence of spectral gaps above the ground state energy (uniformly in the particle number), and other quantities of this type. A lot remains to be done.

References

[1] N.N. Bogoliubov, *On the theory of superfluidity*, J. Phys. (U.S.S.R.) **11**, 23 (1947).

[2] E. Buffet, J.V. Pulè, *Fluctuation properties of the imperfect Bose gas*, J. Math. Phys. **24**, 1608–1616 (1983).

[3] F.J. Dyson, *Ground-State Energy of a Hard-Sphere Gas*, Phys. Rev. **106**, 20–26 (1957).

[4] F.J. Dyson, E.H. Lieb, B. Simon, *Phase Transitions in Quantum Spin Systems with Isotropic and Nonisotropic Interactions*, J. Stat. Phys. **18**, 335–383 (1978).

[5] J. Fröhlich, B. Simon, T. Spencer, *Infrared Bounds, Phase Transitions and Continuous Symmetry Breaking*, Commun. Math. Phys. **50**, 79–85 (1976).

[6] A. Giuliani, R. Seiringer, *The Ground State Energy of the Weakly Interacting Bose Gas at High Density*, J. Stat. Phys. **135**, 915–934 (2009).

[7] T.D. Lee, C.N. Yang, *Many body problem in quantum mechanics and quantum statistical mechanics*, Phys. Rev. **105**, 1119–1120 (1957). T.D. Lee, K. Huang, C.N. Yang, *Eigenvalues and Eigenfunctions of a Bose System of Hard Spheres and Its Low-Temperature Properties*, Phys. Rev. **106**, 1135–1145 (1957).

[8] M. Lewin, R. Seiringer, *Strongly correlated phases in rapidly rotating Bose gases*, J. Stat. Phys. **137**, 1040–1062 (2009).

[9] E.H. Lieb, R. Seiringer, *Proof of Bose-Einstein Condensation for Dilute Trapped Gases*, Phys. Rev. Lett. **88**, 170409 (2002).

[10] E.H. Lieb, R. Seiringer, *Derivation of the Gross-Pitaevskii Equation for Rotating Bose Gases*, Commun. Math. Phys. **264**, 505–537 (2006).

[11] E.H. Lieb, R. Seiringer, J.P. Solovej, *Ground-state energy of the low-density Fermi gas*, Phys. Rev. A **71**, 053605 (2005).

[12] E.H. Lieb, R. Seiringer, J.P. Solovej, J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, Oberwolfach Seminars, Vol. 34, Birkhäuser (2005). Also available at arXiv:cond-mat/0610117.

[13] E.H. Lieb, R. Seiringer, J. Yngvason, *Bosons in a trap: A rigorous derivation of the Gross-Pitaevskii energy functional*, Phys. Rev. A **61**, 043602 (2000).

[14] E.H. Lieb, R. Seiringer, J. Yngvason, *Yrast line of a rapidly rotating Bose gas: Gross-Pitaevskii regime*, Phys. Rev. A **79**, 063626 (2009).

[15] E.H. Lieb, J. Yngvason, *Ground State Energy of the low density Bose Gas*, Phys. Rev. Lett. **80**, 2504–2507 (1998).

[16] E.H. Lieb, J. Yngvason, *The Ground State Energy of a Dilute Two-dimensional Bose Gas*, J. Stat. Phys. **103**, 509 (2001).

[17] O. Penrose, L. Onsager, *Bose-Einstein Condensation and Liquid Helium*, Phys. Rev. **104**, 576–584 (1956).

[18] R. Seiringer, *Ground state asymptotics of a dilute, rotating gas*, J. Phys. A: Math. Gen. **36**, 9755–9778 (2003).

[19] R. Seiringer, *The Thermodynamic Pressure of a Dilute Fermi Gas*, Commun. Math. Phys. **261**, 729–758 (2006).

[20] R. Seiringer, *Free Energy of a Dilute Bose Gas: Lower Bound*, Commun. Math. Phys. **279**, 595–636 (2008).

[21] R. Seiringer, D. Ueltschi, *Rigorous upper bound on the critical temperature of dilute Bose gases*, Phys. Rev. B **80**, 014502 (2009).

[22] D. Ueltschi, *Feynman cycles in the Bose gas*, J. Math. Phys. **47**, 123303 (2006).

[23] H.-T. Yau, J. Yin, *The Second Order Upper Bound for the Ground Energy of a Bose Gas*, J. Stat. Phys. **136**, 453–503 (2009).

[24] J. Yin, *Free Energies of Dilute Bose gases*, preprint, arXiv:0906.1322