

Bose-Einstein condensation and the Simplified Approach to interacting Bosons

Ian Jauslin

Department of Mathematics, Rutgers University

ian.jauslin@rutgers.edu

Abstract

These are lecture notes for a short course on the Simplified Approach to interacting Bosons. We discuss properties of systems of many interacting Bosons, such as gasses of Helium atoms. We pay special attention to the phenomenon of Bose-Einstein condensation, which is a quantum phase in which a positive fraction of particles are all in the same state. We first give an overview of Bose-Einstein condensation in non-interacting systems. Next, we introduce the Simplified Approach, and prove some of its properties.

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1. Introduction

This course is about systems of many interacting Bosons. The first question that we will address is: why should we study interacting Bosons in the first place? Our answer is threefold. First, Bosons exist, and if we want to understand the natural world, we are going to have to study them. Second, systems of many interacting Bosons exhibit interesting and non-trivial physical behavior. Third, they are very challenging to study mathematically, which means that we need to develop new mathematical tools. Let us expand on each of these points.

1 - One of the great successes of science is the understanding that matter is made of particles, and the properties of matter can be understood from the microscopic dynamics of the underlying particles. But can we actually do this? The branch of physics that addresses this question is statistical mechanics, which aims to compute the behavior of matter starting from the microscopic laws of motion guiding its constituents particles. These laws of motion are quantum mechanical, and, in quantum mechanics there are two types of particles: Fermions (such as electrons, protons, neutrinos, etc) or Bosons (such as Helium atoms, photons, Higgs particles, etc). Here, we will focus on Bosons. A good example to keep in mind throughout this course is a gas of Helium atoms in a container. So Bosonic systems exist.

2 - Helium has many interesting properties, but perhaps the most intriguing is that, when the temperature is small enough (below 2K, that is, -271°C or -456°F), it forms a superfluid phase, which looks like a liquid phase, but it can flow without any viscosity, which leads to some fairly surprising behaviors. For instance, when a superfluid is put into a container, capillary forces attract it to the edges of the container, but, since there is no viscosity to compensate for them, these forces pull the superfluid all the way up the wall and trickling down the sides. Another interesting aspect of superfluidity is that classical models do not exhibit superfluidity, so this phase is intrinsically quantum.

Superfluids are very interesting, but not so simple to study. Instead, we will simplify things and focus on a different, but also inherently quantum phase: the Bose-Einstein condensate. This phase was first predicted by Bose [Bo24] and Einstein [Ei24] nearly a century ago, and occurs when most of the particles are all in the same quantum state. In other words, most of the particles are doing the same thing at the same time. As the superfluid phase, this phenomenon does not occur for classical particles, so this is an inherently quantum phase. In fact, it seems somewhat related to the superfluid: if the particles are doing the same thing, why would there be viscosity? (The actual picture is much more complicated than that however.)

Thus, systems of many Bosons exhibit non-trivial physical behavior.

3 - Bose-Einstein condensation has had a resurgence in popularity after 1995, when it was first observed experimentally [AEe95, DMe95]. In particular, the mathematical physics

community set off to solve an important problem: the works of Bose and Einstein are done in a much simplified model, in which particles are assumed not to interact with each other. This makes things much simpler: if the particles are independent, it suffices to understand how a single particle behaves, since the situation is identical for all the others. However, in the presence of interactions, no one has yet been able to prove that Bose-Einstein condensation even occurs (and real Bosonic systems have interactions, except for photons, but for those, we don't even know how to write down an appropriate wave equation [Op31]). (Here, the word “prove” is key: most everyone accepts Bose-Einstein condensation occurs in interacting systems, but we don't have a mathematical proof yet.) In fact, before 1998, there was no complete mathematical handle on pretty much any of the properties of interacting Bosonic gasses. In 1998, Lieb and Yngvason [LY98] computed the asymptotic behavior at low density of the ground-state energy (see (3.30)) and this started a flurry of activity. Back in 1957, Lee, Huang and Yang [LHY57] had made a series of predictions, one of which was a low-density expansion for the ground-state energy that went one step further than what Lieb and Yngvason proved in 1998. The mathematical physics community rose to the challenge, and embarked upon a twenty year effort to prove the Lee-Huang-Yang formula. This was finally accomplished in 2020, after a long series of works culminating in [YY09, FS20, BCS21, FS23].

However, these successes only concern the ground-state energy. In particular, there still is no proof of Bose-Einstein condensation. The results on the ground-state energy were obtained by finding a robust mathematical basis for *Bogolyubov theory*. Bogolyubov theory [Bo47] is an approach that was introduced by Bogolyubov in the 1940's to understand the low-density properties of Bose gasses. One can do a lot with Bogolyubov theory, and many predictions can be made from it [LHY57]. However, to this day, only its approach to the ground-state energy has been made rigorous.

In this course, we will present a different approach, called the *Simplified Approach*. The Simplified Approach was first introduced by Lieb in 1963 [Li63], but after a short series of papers by Lieb and coauthors [LS64, LL64], it has largely been forgotten. We have recently had a fresh look at this approach, in a collaboration with Carlen and Lieb [CJL20, CJL21, CHe21, Ja22, Ja23b, Ja23] and found that the predictions of the Simplified Approach far exceeded our expectations. Indeed, we found that it is as good as Bogolyubov theory at low densities [CJL20, CJL21] (at least as far as the ground state is concerned), it also reproduces the behavior of the Bose gas at high densities [CJL20]. We have even found very good agreement for some systems *over the entire range of densities* [CHe21, Ja23].

The Simplified Approach consists in replacing the original problem that involves an infinite number of particles with a non-linear, non-local equation for a single particle. This is a familiar approach in physics, where many-body problems are replaced with non-linear effective equations. The Simplified Approach actually gives us several levels of approximation, and defines a family of equations that are more or less accurate, and correspondingly, harder or easier to solve. Some can be studied analytically, whereas others are only really amenable to a numerical analysis.

In conclusion, systems of many interacting Bosons are interesting: they exist, are physically non-trivial, and mathematically challenging.

Outline:

We will start out this course with a discussion of Bose-Einstein condensation in non-interacting systems, see Section 2. The arguments presented there follow the original derivation by Bose and Einstein [Bo24, Ei24]. The discussion will begin with a much abbreviated introduction to quantum statistical mechanics. Next, we will present the Simplified Approach, see Section 3. In that section, we will also present the conjectures on the Bose gas that the Simplified Approach was

developed to address. In doing so, we will give an overview of scattering theory, which underlies the intuition in the low-density regime. Some of the more abstract mathematical results needed for this section have been deferred to Appendices A1 and A2. Finally, in Section 4, we discuss some open problems. There are also some exercises at the very end of this document.

2. Bose-Einstein condensation

Bose-Einstein condensation serves as the main motivation for the discussion in this course. Proving the existence of Bose-Einstein condensation in interacting systems is the main open problem in the field, and the principle reason for the entire discussion that follows this section is to try new ways of approaching that. In this section, we will discuss what Bose-Einstein condensation is in more detail, and prove that it occurs in a much simplified model: non-interacting Bosons. But first, we must define what a “Boson” is, as well as the model we will be using.

2.1. Elements of quantum statistical mechanics

One of the great achievements of modern science is the understanding that macroscopic matter is made of microscopic elementary particles, and that the properties of the whole stem from the interaction between these elementary particles. The goal of statistical mechanics is to understand how this works, that is, the relation between the microscopic and the macroscopic worlds.

2.1.1. Classical statistical mechanics

Let us think classically for the moment. Classical particles are governed by Newton’s second law of motion: $F = ma$. In the case of conservative systems (at their deepest level, all systems are actually conservative: friction is an effective description of a complicated, conservative behavior), this can be restated in the Hamiltonian formalism. If I have N particles, the Hamiltonian is a function on a $6N$ -dimensional manifold (think \mathbb{R}^{6N} for simplicity) that may look something like this:

$$H_N(x_1, \dots, x_N; p_1, \dots, p_N) = \sum_{i=1}^N \frac{1}{2m} p_i^2 + \sum_{1 \leq i < j \leq N} v(x_i - x_j) \quad (2.1)$$

in which $x_i \in \mathbb{R}^3$ and $p_i \in \mathbb{R}^3$ are the positions and momenta of the particles, and v is a pair interaction potential. This dictates the *microscopic* dynamics. But what if we were to use this formalism to understand the properties of a gas of particles? Say we want to compute the pressure and temperature in a room full of air. In your average room, there will be $N = 10^{24}$ particles, that’s a trillion trillion particles. The Hamiltonian picture gives us a trajectory for each of these particles. This is an incredibly uselessly large amount of information, if all we were after in the first place was pressure and temperature.

Instead, we will approach the problem statistically: instead of following each individual particles, let us compute average behaviors. The question is: average with respect to what probability measure? Here, things get complicated, and, in the interest of time, let us just say that there are three satisfactory measures to consider, that are called the *microcanonical*, *canonical* and *grand-canonical* measures. In this section we’ll focus on the grand-canonical measure. In this setting, there are two parameters: the *temperature* $T > 0$ (yes, in this formalism, temperature is a parameter) and the *chemical potential* $\mu \in \mathbb{R}$. Given these two, the probability of a given configuration $(x_1, \dots, x_N; p_1, \dots, p_N)$ with N particles is

$$\frac{1}{\Xi} e^{-\beta H_N(x_1, \dots, x_N; p_1, \dots, p_N) + \beta \mu N} \quad (2.2)$$

where

$$\beta = \frac{1}{k_B T} \quad (2.3)$$

in which k_B is the *Boltzmann constant* and Ξ is a normalization:

$$\Xi := 1 + \sum_{N=1}^{\infty} \frac{1}{N!} \int dx_1 \cdots dx_N dp_1 \cdots dp_N e^{-\beta H_N(x_1, \dots, x_N; p_1, \dots, p_N) + \beta \mu N}. \quad (2.4)$$

We immediately notice an issue: if the x_i take values anywhere in \mathbb{R}^3 , Ξ will come out infinite! To avoid this, let us restrict $x_i \in [0, L]^3$ for some finite L , and, later one, we will take $L \rightarrow \infty$. Note that Ξ involves a sum over N : in the grand-canonical picture, we consider all possible numbers of particles. In addition, note the $1/N!$ factor, which indicates that all the particles are identical, so the labelling $i = 1, \dots, N$ should not affect the statistics!

Why do we choose a probability of the form (2.2)? The real reason is that it is compatible with the laws of thermodynamics [Ru99, Ga99], but that is a discussion for another time. Instead, let us have a look at the properties of this distribution, and check that they make sense. The first term in the exponential is $e^{-\beta H}$, and, since $\beta > 0$, it says that configurations with large energies will be less likely. The parameter β (the temperature) quantifies how much less likely. This is rather sensible: we know that energy tends to be minimized, and that this is more true at low temperatures than higher ones. The second term is $e^{\beta \mu N}$ controls the number of particles. If $\mu > 0$, then configurations with more particles are more likely, whereas $\mu < 0$ makes more particles unlikely. Thus the chemical potential μ controls the *density* of particles.

Why do we use the chemical potential instead of simply fixing the number of particles (which is, after all, the most direct way of setting the density)? This can be done: in statistical mechanics, the situation in which the number of particles is fixed is called the *canonical formalism*. The parameters are then the temperature and the number of particles. One can show that the two formalisms are equivalent: there exists a mapping between the density and chemical potential that makes all average observables identical in both formalisms. However, in certain situations, it may be easier to compute these averages in one formalism rather than the other. In the case of Bose-Einstein condensation, the computation is easy in the grand-canonical, and impossibly difficult in the canonical, which is why we use the chemical potential instead of the density.

Thinking probabilistically in this manner, we can then compute the average behavior of these particles, and compute properties for the macroscopic system. More specifically, we define an *observable* A as a map from \mathbb{N} (the number of particles) to functions on the phase space with N particles: $A_N(x_1, \dots, x_N; p_1, \dots, p_N)$. The average of an observable A is

$$\langle A \rangle = \frac{1}{\Xi} \left(A_0 + \sum_{N=1}^{\infty} \frac{1}{N!} \int dx_1 \cdots dx_N dp_1 \cdots dp_N A_N(x_1, \dots, x_N; p_1, \dots, p_N) e^{-\beta H_N(x_1, \dots, x_N; p_1, \dots, p_N) + \beta \mu N} \right). \quad (2.5)$$

An example of an observable could be the number of particles itself:

$$\mathcal{N}_N := N \quad (2.6)$$

or the total energy

$$\mathcal{E}_N(x_1, \dots, x_N; p_1, \dots, p_N) := H_N(x_1, \dots, x_N; p_1, \dots, p_N). \quad (2.7)$$

2.1.2. Quantum statistical mechanics

We have thus defined the grand-canonical ensemble for systems of classical particles. What about quantum particles? The microscopic state of a system of quantum particles is given by a wavefunction, for instance, $\psi \in L_2(\mathbb{R}^3)^{\otimes N}$, and the dynamics is given by a Hamiltonian operator, for instance,

$$H_N = - \sum_{i=1}^N \frac{1}{2m} \Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j) \quad (2.8)$$

where Δ_i is the Laplacian with respect to x_i . (Throughout this document, we choose units so that $\hbar = 1$; we keep track of the mass because different authors use $m = 1$ or $m = 1/2$, so we keep it to avoid confusion.) This is the microscopic description of the system. Similarly to the classical case, to treat situations with a huge number of particles, we will approach the system statistically. In the classical case, we considered a probability distribution over all possible configurations, without fixing the number of particles. Here, we wish to do the same. The configurations are wavefunctions, which, again, are in $L_2(\mathbb{R}^3)^{\otimes N}$. Instead of integrating over configurations as we did in the classical case, we will take traces over $L_2(\mathbb{R}^3)^{\otimes N}$.

There is just one subtlety here: the particles are indistinguishable. In the classical setting, this is dealt with simply by adding a $1/N!$ that accounts for the fact that configurations that are permutations of each other are really identical. In the quantum mechanical case, however, the notion of ‘‘identical’’ is more complicated: two wavefunctions that have the same absolute value, but a different phase, are indistinguishable. Therefore, to enforce the fact that particles are indistinguishable, it suffices to consider wavefunctions whose absolute value does not change under exchanges of particles, but these permutations of particles may lead to a different phase. As it turns out, there are only two possible phase shifts that are consistent in three dimensions: one possibility is the trivial one, in which wavefunctions are symmetric under exchanges of particles: for any permutation $\sigma \in \mathcal{S}_N$,

$$\psi_{\text{sym}}(x_1, \dots, x_N) = \psi_{\text{sym}}(x_{\sigma(1)}, \dots, x_{\sigma(N)}) \quad (2.9)$$

and the other is that exchanging two particles leads to the wavefunction changing sign:

$$\psi_{\text{antisym}}(x_1, \dots, x_N) = (-1)^\sigma \psi_{\text{antisym}}(x_{\sigma(1)}, \dots, x_{\sigma(N)}). \quad (2.10)$$

Why are these the only two possibilities (in three dimensions)? Mathematically, this comes from the fact that there are only two irreducible representations of the permutation group in three dimensions. More intuitively, if two particles are exchanged, the wavefunction should pick up a phase $e^{i\theta}$, but if I exchange the particles back, we should return to the original wavefunction, and thus $e^{2i\theta} = 1$ and so θ is either 0 or π . (This is not the case in two dimensions, for reasons we will not elaborate here.)

We therefore define the symmetric subspace:

$$L_{2,\text{sym}}^{(N)}(\mathbb{R}^3) := \{\psi \in L_2(\mathbb{R}^3)^{\otimes N} : \forall \sigma \in \mathcal{S}_N, \psi(x_1, \dots, x_N) = \psi(x_{\sigma(1)}, \dots, x_{\sigma(N)})\} \quad (2.11)$$

and the antisymmetric subspace:

$$L_{2,\text{antisym}}^{(N)}(\mathbb{R}^3) := \{\psi \in L_2(\mathbb{R}^3)^{\otimes N} : \forall \sigma \in \mathcal{S}_N, \psi(x_1, \dots, x_N) = (-1)^\sigma \psi(x_{\sigma(1)}, \dots, x_{\sigma(N)})\}. \quad (2.12)$$

Note that the symmetric and antisymmetric subspaces span all of L_2 :

$$L_2(\mathbb{R}^3)^{\otimes N} = L_{2,\text{sym}}^{(N)}(\mathbb{R}^3) \oplus L_{2,\text{antisym}}^{(N)}(\mathbb{R}^3). \quad (2.13)$$

Now, from a physical point of view, systems of many indistinguishable particles come in two flavors: those with symmetric wavefunctions and those with antisymmetric wavefunctions. Symmetric ones are called *Bosons* and antisymmetric ones are called *Fermions*. (Another way of

seeing this is to think of particles as corresponding to irreducible representations of symmetry groups; the Boson/Fermion distinction corresponds to the two irreducible representations of the permutation group.) Electrons, protons, quarks are examples of Fermions. Photons, Helium atoms, Higgs particles are examples of Bosons. Here, we will consider systems of many Bosons, which is to say that the configuration space we will consider is $L_{2,\text{sym}}^{(N)}(\mathbb{R}^3)$.

An observable in the quantum setting is a map A from \mathbb{N} (the number of particles) to a self-adjoint operator A_N on $L_{2,\text{sym}}^{(N)}(\mathbb{R}^3)$. An example of an observable is the number of particles operator:

$$\mathcal{N}_N \psi := N \psi \quad (2.14)$$

another is the total energy: H_N . The average of an observable is then defined as

$$\langle A \rangle := \frac{1}{\Xi} \left(A_0 + \sum_{N=1}^{\infty} \text{Tr}_{L_{2,\text{sym}}^{(N)}(\mathbb{R}^3)} (A_N e^{-\beta H_N + \beta \mu \mathcal{N}_N}) \right) \quad (2.15)$$

with

$$\Xi := 1 + \sum_{N=1}^{\infty} \text{Tr}_{L_{2,\text{sym}}^{(N)}(\mathbb{R}^3)} (e^{-\beta H_N + \beta \mu \mathcal{N}_N}). \quad (2.16)$$

As in the classical case, we immediately notice an issue: the trace in Ξ is infinite! To prevent this we replace \mathbb{R}^3 with $[0, L]^3$:

$$\Xi := 1 + \sum_{N=1}^{\infty} \text{Tr}_{L_{2,\text{sym}}^{(N)}([0, L]^3)} (e^{-\beta H_N + \beta \mu \mathcal{N}_N}). \quad (2.17)$$

2.2. The ideal Bose gas

Let us now apply these concepts to the non-interacting (a.k.a. the ideal) Bose gas. The Hamiltonian is

$$H_N = - \sum_{i=1}^N \frac{1}{2m} \Delta_i. \quad (2.18)$$

We will consider this system on the cube $[0, L]^3$ with periodic boundary conditions (other boundary conditions can be treated similarly). In other words, we replace \mathbb{R}^3 with $\mathbb{T}^3 := (\mathbb{R}/(L\mathbb{Z}))^3$. This Hamiltonian is easily diagonalized: the eigenvectors of $\frac{1}{2m} \Delta$ are plane waves:

$$e^{ikx}, \quad k \in \frac{2\pi}{L} \mathbb{Z}^3 \quad (2.19)$$

whose eigenvalue is

$$\epsilon_k := \frac{k^2}{2m}. \quad (2.20)$$

We therefore have a (Hilbert) basis, in which each element with N particles is indexed by an unordered sequence of N wavevectors $k \in \frac{2\pi}{L} \mathbb{Z}^3$ (the vectors need not be different). Equivalently, a basis vector can be written as a function that takes a wavevector k and returns the number of particles of that wavevector. This allows us to compute Ξ in the case $\mu < 0$: we write the sum over N of the trace in (2.17) as

$$\Xi = \prod_{k \in \frac{2\pi}{L} \mathbb{Z}^3} \sum_{N_k=0}^{\infty} e^{-\beta(\frac{k^2}{2m} - \mu)N_k} \quad (2.21)$$

In the case $\mu < 0$, this series is absolutely convergent:

$$\Xi = \prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{1 - e^{-\beta(\frac{k^2}{2m} - \mu)}}. \quad (2.22)$$

Let us now compute some observables. Let \mathcal{B}_q be the number of particles in the state q whose average is thus easily computed:

$$\langle \mathcal{B}_q \rangle = \frac{1}{\Xi} \left(\sum_{N_q=0}^{\infty} N_q e^{-\beta(\frac{q^2}{2m} - \mu)N_q} \right) \prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3 \setminus \{q\}} \sum_{N_k=0}^{\infty} e^{-\beta(\frac{k^2}{2m} - \mu)N_k} \quad (2.23)$$

and so (see Exercise E1)

$$\langle \mathcal{B}_q \rangle = \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1} \quad (2.24)$$

which is called the *Bose-Einstein distribution*. It is the distribution of particles as a function of the wavevector q .

2.3. Bose-Einstein condensation in the ideal Bose gas

By summing the number of particles of momentum q , we can compute the average total number of particles:

$$\langle \mathcal{N} \rangle = \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3} \langle \mathcal{B}_q \rangle = \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1} \quad (2.25)$$

and the average density:

$$\rho_L(\mu) := \frac{\langle \mathcal{N} \rangle}{L^3} = \frac{1}{L^3} \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1}. \quad (2.26)$$

The density is an important quantity. As was discussed above, the mapping between density and chemical potential is what establishes the equivalence between the grand-canonical and canonical formalisms (which are the points of view with fixed chemical potential and fixed density respectively). Therefore, we will be interested in the mapping $\mu \mapsto \rho_L(\mu)$. But first, let us simplify the expression by taking the $L \rightarrow \infty$ limit.

For fixed $\mu < 0$, this is a Riemann sum, so the limit $L \rightarrow \infty$ turns the sum to an integral (see Exercise E2):

$$\rho(\mu) := \lim_{L \rightarrow \infty} \rho_L(\mu) = \int_{\mathbb{R}^3} \frac{dq}{(2\pi)^3} \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1}. \quad (2.27)$$

By dominated convergence, one easily checks (see Exercise E2) that this is a strictly increasing function of μ . Furthermore, by dominated convergence, (see Exercise E2)

$$\lim_{\mu \rightarrow -\infty} \rho(\mu) = 0 \quad (2.28)$$

and

$$\lim_{\mu \rightarrow 0} \rho(\mu) = \int_{\mathbb{R}^3} \frac{dq}{(2\pi)^3} \frac{1}{e^{\beta\frac{q^2}{2m}} - 1} = \left(\frac{2m}{\beta} \right)^{\frac{3}{2}} \int_{\mathbb{R}^3} \frac{dq}{(2\pi)^3} \frac{1}{e^{q^2} - 1} =: \rho_c(\beta) \quad (2.29)$$

Thus, for $\mu \in (-\infty, 0)$, $\rho(\mu)$ increases from 0 to $\rho_c(\beta)$, which is finite. For $\mu > 0$, the right side of (2.27) is infinite. In particular, proceeding in this way, we only cover a finite range of densities.

What of the densities with $\rho > \rho_c(\beta)$? In other words, can we set the chemical potential μ in such a way that $\rho > \rho_c(\beta)$?

To achieve this, instead of fixing μ and taking $L \rightarrow \infty$, we allow μ to depend on L . To make this clear, we denote μ by μ_L . We will choose μ_L such that $\mu_L \rightarrow 0$ as $L \rightarrow \infty$ (if μ_L stayed converged to a negative value, then we would find the same result as above). Doing so changes the computation in one way: when passing to the $L \rightarrow \infty$ limit, we must pay attention to the $q = 0$ term in the sum. Let us separate it out:

$$\rho_L(\mu_L) = \frac{1}{L^3} \frac{1}{e^{-\beta\mu_L} - 1} + \frac{1}{L^3} \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3 \setminus \{0\}} \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu_L)} - 1}. \quad (2.30)$$

The second term converges uniformly in μ :

$$\frac{1}{L^3} \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu_L)} - 1} \leq \frac{1}{L^3} \frac{1}{e^{\beta \frac{2\pi^2}{mL^2}} - 1} \quad (2.31)$$

which is bounded. Thus, taking the limit $L \rightarrow \infty$,

$$\lim_{L \rightarrow \infty} \rho_L(\mu_L) = \lim_{L \rightarrow \infty} \frac{1}{L^3} \frac{1}{e^{-\beta\mu_L} - 1} + \int_{\mathbb{R}^3} \frac{dq}{(2\pi)^3} \frac{1}{e^{\beta \frac{q^2}{2m}} - 1} \quad (2.32)$$

that is

$$\lim_{L \rightarrow \infty} \rho_L(\mu_L) = \lim_{L \rightarrow \infty} \frac{1}{L^3} \frac{1}{e^{-\beta\mu_L} - 1} + \rho_c(\beta). \quad (2.33)$$

Thus, any density $\rho > \rho_c(\beta)$ can be attained by taking μ_L such that

$$\frac{1}{L^3} \frac{1}{e^{-\beta\mu_L} - 1} = \rho - \rho_c(\beta) \quad (2.34)$$

that is

$$\mu_L = -\frac{1}{\beta} \log \left(1 + \frac{1}{L^3(\rho - \rho_c(\beta))} \right). \quad (2.35)$$

In this case,

$$\lim_{L \rightarrow \infty} \frac{1}{L^3} \langle \mathcal{B}_0 \rangle = \lim_{L \rightarrow \infty} \frac{1}{L^3} \frac{1}{e^{-\beta\mu_L} - 1} = \rho - \rho_c(\beta) \quad (2.36)$$

and for $q \neq 0$,

$$\lim_{L \rightarrow \infty} \frac{1}{L^3} \langle \mathcal{B}_q \rangle = \lim_{L \rightarrow \infty} \frac{1}{L^3} \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu_L)} - 1} = 0. \quad (2.37)$$

Thus, choosing μ_L in this way, we find that the number of particles in the state $q = 0$ is $L^3(\rho - \rho_c)$, that is, the number of particles in this state is proportional to N . There is a *macroscopic* proportion of particles that are all in this one state. Whereas in every other state $q \neq 0$, the fraction of particles is 0.

Let's take a step back. We have been working in the grand-canonical ensemble, that is, with a fixed chemical potential and a variable number of particles. Proceeding in this way, we have computed the average density, and found a bijection between the chemical potential and the density, provided we allow the chemical potential to depend on the size of the system L . This allows us to switch the point of view and consider the system at fixed density and temperature. Thinking in this way, we find that the behavior of the system depends in a non-trivial way on the density. If $\rho < \rho_c(\beta)$, then $\langle \mathcal{B}_0 \rangle / L^3 \rightarrow 0$, but if $\rho > \rho_c(\beta)$, then $\langle \mathcal{B}_0 \rangle / L^3 \rightarrow c_0 > 0$, see Figure-2.1. Or, to put it into words, for small densities, the system behaves like a regular, classical gas, but when the density exceeds $\rho_c(\beta)$, a huge number of particles all occupy the same state. This phenomenon is called Bose-Einstein condensation.

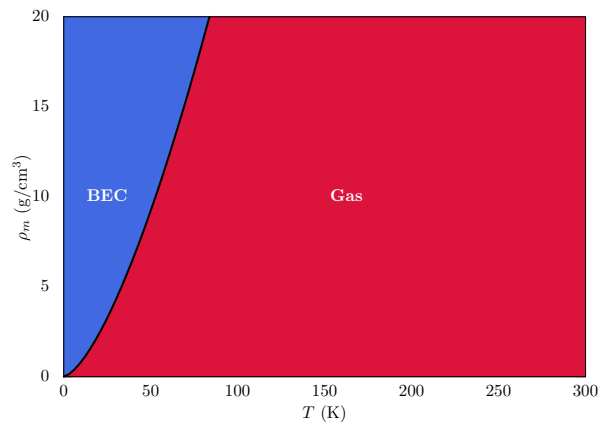


fig 2.1: The phase diagram of the ideal gas of Helium-4 atoms. The y -axis is the mass density.

This is significant for several reasons. For one, this is a new phase of matter that is uniquely quantum: classical systems do not behave like this. In addition, Bose-Einstein condensation may be the underlying mechanism for some truly astonishing phenomena: superfluidity and superconductivity. Fluids flow, and, while doing so, they lose energy to friction. This is visible in everyday life through the concept of *viscosity*. A superfluid has zero viscosity, which means that it can flow without any friction. This leads to truly astonishing behaviors: flows can separate and recombine without any losses, which allows superfluids to flow through membranes that are completely water-tight for ordinary fluids. In addition, because no energy is lost through viscosity, the capillary force becomes dominant, and superfluids can be seen to creep up the sides of any container they are put in and escape. This is fun and non-trivial behavior, but it also comes with serious technological applications. The most astonishing of which may be superconductivity. Electrical currents are caused by electrons flowing through metals. As they do so, they are slowed by resistance, and the metal heats up. Superconductivity is a phenomenon by which electrons can flow through a metal *without resistance*. In most applications, resistance is waste, which makes superconducting metals extremely useful in many applications. One way to understand the phenomenon is that electrons pair up into an effective excitation called a *Cooper pair*. Now an electron is a Fermion, but a pair of electrons is a Boson, so Cooper pairs are Bosonic. If these form the analogue of a superfluid phase, they can move around without resistance. But what does all this have to do with Bose-Einstein condensation? The answer is not so straightforward, but it has been posited that Bose-Einstein condensation is the underlying mechanism for both superfluidity and superconductivity. This can be understood intuitively: if most particles are in the same state, they are all doing the same thing, and since friction comes from colliding particles, friction can disappear. (This is a very handwavy explanation: the actual relation between Bose-Einstein condensation, superfluidity and superconductivity is a rather difficult subject).

Bose-Einstein condensation was first predicted by Bose [Bo24] and Einstein [Ei24] in the 1920's (following roughly the argument given above). It took until 1995 before it was finally observed experimentally [AEe95, DMe95]. The experiments consist in trapping very cold Bosonic atoms (rubidium and sodium) at a high enough density so as to be in the Bose-Einstein condensate phase. The trap is then released, and the momentum of the atoms measured. The result is a sharply peaked distribution: many atoms were in the same state!

3. The Simplified Approach

3.1. Interacting Bose gasses

We have proved that the ideal Bose gas exhibits Bose-Einstein condensation. The approach we took consisted in computing exact expressions for the partition function Ξ and the average occupation numbers $\langle \mathcal{B}_q \rangle$. We were able to do this because the ideal Bose gas is an “exactly solvable model”, but this is a very special feature of that specific model. Furthermore, the ideal gas is not very realistic: there are no interactions between particles, which is not how real matter behaves. Let us consider a more realistic Hamiltonian:

$$H_N = - \sum_{i=1}^N \frac{1}{2m} \Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j) \quad (3.1)$$

where v is the potential that accounts for the interaction between pairs of particles. (Throughout this document, we choose units so that $\hbar = 1$; we keep track of the mass because different authors use $m = 1$ or $m = 1/2$, so we keep it to avoid confusion.) This potential could be the Coulomb potential $1/|x|$ for charged particles, or the Lennard-Jones potential for interacting atoms, or something more realistic that accounts for the fine structure of atoms. Here, we will restrict our focus a bit and assume that v is integrable ($v \in L_1(\mathbb{R}^3)$) and non-negative: $v(x) \geq 0$. In addition, we will only consider the zero-temperature state ($T = 0$ that is $\beta = \infty$), in other words, we will be considering only the ground state of H_N , which is the eigenstate with lowest eigenvalue. Ultimately, we would like to study the system at positive temperatures, but, as we will see, the zero-temperature analysis is difficult enough.

Adding the potential breaks the exact solvability of the model: there no longer is an exact expression for the observables associated to this Hamiltonian, so we will have to proceed differently. However, as of this writing, there are no tools to compute very much for this model. The only rigorous results are computations of the average energy for small [YY09, FS20] or large [Li63] densities. In particular, there is no proof of Bose-Einstein condensation.

If we can't solve this model, what can we do? One approach is to change the model. For instance, we could make the potential depend on the number of particles. This is not very realistic for a microscopic model, but it can accurately capture the behavior of the system in certain asymptotic regimes. Specifically, the Gross-Pitaevskii scaling, which consists in taking the potential to be

$$v(x) \mapsto N^{\frac{2}{3}} v(N^{\frac{1}{3}} x) \quad (3.2)$$

corresponds to an infinitely dilute gas $\rho = 0$, and the mean-field scaling

$$v(x) \mapsto \frac{1}{N^{\frac{5}{3}}} v(N^{-\frac{1}{3}} x) \quad (3.3)$$

corresponds to an infinitely dense system $\rho = \infty$. Both regimes have been studied extensively [Sc22, Se11] and much has been proved about these. However, these scaling regimes are too idealized to capture the real physical behavior of the system at finite density.

Another approach is to make some approximations that, while not being exact, capture some of the physical behavior of the system. In a sense, the ideal Bose gas is such an approximation. However, the potential changes things, so a more refined approximation is in order. One such approximation was introduced by Bogolyubov [Bo47] and has been studied extensively since then. It has since become known as *Bogolyubov theory*. The key observation made by Bogolyubov is that the behavior of the particles in the condensate is simple, we can deal with them in a simplified way (this idea is rigorous), and that what is left-over does not interact too much so we can drop all the interaction terms in the Hamiltonian that we don't know how to deal with. This idea seems

to work very well as long as the density is small enough (but not 0 as for the Gross-Pitaevskii scaling). One distinct advantage is that, after having ignored certain terms, the model becomes exactly solvable like the ideal Bose gas, so everything can be computed. This is what was done by Lee, Huang and Yang [LHY57], who thus made a number of predictions about the interacting Bose gas, concerning the energy, condensate fraction and two point correlation function. In all of these, the effect of the interaction appears through a quantity called the *scattering length*. Before stating the conjectures of Lee, Huang and Yang, let us discuss the scattering length.

3.2. Scattering theory

The physical picture that underlies Bogolyubov theory is that, at low densities, the behavior of the system should be dominated by single body dynamics, and the interaction only comes in in the rare events when particles get close to each other. Because these are rare, these interaction events will only involve single pairs of particles. These pair interaction events are called *scattering events*. The physical picture to have in mind is two particles coming closer together in a straight line (a free state), interacting, and leaving in a different free state than they started in. By translation invariance, we can work in the center of mass reference frame, in which the scattering event can be seen as a single particle flying through a fixed potential. The Schrödinger equation for this process is

$$-\frac{1}{m}\Delta\psi + v(x)\psi = i\partial_t\psi \quad (3.4)$$

(note the absence of a 1/2 factor in front of the Laplacian which comes from the fact that the effective mass in the center of mass frame is $\frac{m_1 m_2}{m_1 + m_2} = m/2$.) (Recall that we chose units so that $\hbar = 1$.)

We will focus on stationary solutions of the equation:

$$-\frac{1}{m}\Delta\psi + v(x)\psi = E\psi \quad (3.5)$$

and will study spherically symmetric solutions, which must have $E = 0$ (this is an *s-wave*). That is, we will solve the *scattering equation*

$$-\frac{1}{m}\Delta\psi + v(x)\psi = 0. \quad (3.6)$$

We impose the boundary condition

$$\lim_{|x|\rightarrow\infty} \psi(x) = 1. \quad (3.7)$$

Let us consider a simple example: the hard core potential:

$$v(x) = \begin{cases} 0 & \text{if } |x| > R \\ \infty & \text{otherwise.} \end{cases} \quad (3.8)$$

In other words, the scattering equation is

$$\begin{cases} \psi(x) = 0 & \text{if } |x| \leq R \\ -\frac{1}{m}\Delta\psi = 0 & \text{otherwise.} \end{cases} \quad (3.9)$$

In spherical coordinates, assuming ψ is spherically symmetric, that is, it only depends on $r \equiv |x|$,

$$\Delta\psi = \frac{1}{r}\partial_r^2(r\psi) \quad (3.10)$$

so $\Delta\psi = 0$ is

$$r\psi = cr - a \quad (3.11)$$

and so, for $r > R$,

$$\psi = c - \frac{a}{r} \quad (3.12)$$

and, using $\psi(R) = 0$ and $\psi \rightarrow 1$,

$$c = 1, \quad a = R \quad (3.13)$$

so

$$1 - \psi = \frac{R}{r}. \quad (3.14)$$

The constant c is dimensionless, and the constant a has the dimension of a length. In this example, we see that a is the radius of the potential.

Let us now turn to a different potential: the soft core potential:

$$v(x) = \begin{cases} 0 & \text{if } |x| > R \\ U & \text{otherwise} \end{cases} \quad (3.15)$$

with $U > 0$. The scattering equation is thus

$$\begin{cases} -\frac{1}{m}\Delta\psi + U\psi = 0 & \text{if } |x| \leq R \\ -\frac{1}{m}\Delta\psi = 0 & \text{otherwise} \end{cases} \quad (3.16)$$

which, in spherical coordinates is

$$\begin{cases} -\frac{1}{mr}\partial_r^2(r\psi) + U\psi = 0 & \text{if } |x| \leq R \\ -\frac{1}{mr}\partial_r^2(r\psi) = 0 & \text{otherwise.} \end{cases} \quad (3.17)$$

The solution is (see Exercise E4), using the fact that $r\psi$ should equal 0 at $r = 0$ and that $r\psi$ is continuous at $r = R$,

$$r\psi = \begin{cases} (R - a)\frac{\sinh(\sqrt{Um}r)}{\sinh(\sqrt{Um}R)} & \text{if } r \leq R \\ r - a & \text{otherwise} \end{cases} \quad (3.18)$$

with

$$a = R - \frac{\tanh(\sqrt{Um}R)}{\sqrt{Um}}. \quad (3.19)$$

Note that a is an increasing function of U , ranging from 0 for $U = 0$ to R at infinity. Therefore, the solution of the scattering equation for large r looks like that of a hard core, but with radius a instead of R .

This length scale a is called the *scattering length*. We can define it for potentials that are compactly supported, that is, for which there exists R such that $v(x) = 0$ for $|x| > R$. In this case, for $|x| > R$,

$$\psi(x) = 1 - \frac{a}{|x|} \quad (3.20)$$

where a is the scattering length. Alternatively, the scattering length can be computed as follows.

Lemma 3.1

If v is spherically symmetric, compactly supported and integrable, then

$$a = \frac{m}{4\pi} \int dx v(x)\psi(x). \quad (3.21)$$

Proof: By the scattering equation (3.6),

$$\frac{m}{4\pi} \int dx v(x)\psi(x) = \frac{1}{4\pi} \int dx \Delta\psi(x) \quad (3.22)$$

which we rewrite in spherical coordinates, using $\Delta\psi = \frac{1}{r^2}\partial_r(r^2\partial_r\psi)$:

$$\frac{m}{4\pi} \int dx v(x)\psi(x) = \int_0^\infty dr \partial_r(r^2\partial_r\psi(r)) = \lim_{R \rightarrow \infty} \int_0^R dr \partial_r(r^2\partial_r\psi(r)) = \lim_{R \rightarrow \infty} R^2\partial_r\psi(R). \quad (3.23)$$

Since v has compact support, $v(x) = 0$ for $|x| > R$, so

$$\psi = 1 - \frac{a}{r} \quad (3.24)$$

and

$$\partial_r\psi = \frac{a}{r^2} \quad (3.25)$$

so

$$\lim_{R \rightarrow \infty} R^2\partial_r\psi(R) = a \quad (3.26)$$

which proves the lemma. □

This lemma gives us an alternative definition of the scattering length, which does not require v to be compactly supported, just that it be in $L_1(\mathbb{R}^3)$ so that the integral is finite.

3.3. The Lee-Huang-Yang predictions

By following the prescriptions of Bogolyubov theory, Lee, Huang and Yang [LHY57] made a number of predictions about the ground state (zero-temperature state) of the interacting Bose gas. Here, we will focus on their predictions for the energy per particle, the condensate fraction and the two-point correlation function.

As was mentioned above, we study the ground state of the Hamiltonian (3.1). Let us be more specific. As we did in section 2, we will consider the system to be in a finite volume with periodic boundary conditions. We denote the volume by V , and place the particles on the torus $\mathbb{R}^3/(V^{\frac{1}{3}}\mathbb{Z})^3$. Unlike section 2, we will work in the canonical ensemble, which means that we fix the number of particles to some $N \in \mathbb{N}$. We will be interested in the *thermodynamic limit*, in which

$$N \rightarrow \infty, \quad V \rightarrow \infty, \quad \frac{N}{V} = \rho \quad (3.27)$$

with ρ (the density) fixed. In this case, the Hamiltonian (3.1) has pure-point spectrum (by Theorem A1.11, e^{-H_N} is compact, so it has discrete spectrum, and therefore so does H_N). Its lowest eigenvalue is denoted by E_0 , and is called the *ground-state energy*. The corresponding eigenvector is denoted by ψ_0 :

$$H_N\psi_0 = E_0\psi_0. \quad (3.28)$$

(Note that the ground state is unique, see Exercise E5.)

The ground-state energy per particle is defined as

$$e_0 := \lim_{\substack{N, V \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{E_0}{N}. \quad (3.29)$$

Lee, Huang and Yang predicted the following low-density expansion for the ground state energy.

Conjecture 3.2

[LHY57, (25)] For any potential $v \in L_1(\mathbb{R}^3)$ with $v \geq 0$ (actually, the potential may include a hard-core component), as $\rho \rightarrow 0$,

$$e_0 = \frac{2\pi}{m} \rho a \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a^3} + o(\sqrt{\rho}) \right) \quad (3.30)$$

where a is the scattering length of the potential, and

$$\lim_{\rho \rightarrow 0} \frac{o(\sqrt{\rho})}{\sqrt{\rho}} = 0. \quad (3.31)$$

The first two orders of this expansion thus only depend on the potential through its scattering length. This is a universality result: any two potentials that share the same scattering length, even if they are radically different, will yield the same first two orders of the low-density expansion of the ground state energy.

The condensate fraction is the fraction of particles that are in the Bose-Einstein condensate. In the case of the ideal Bose gas, the particles condensed in the $k = 0$ state, which is the constant wavefunction. In the interacting case, the condensate state will still be the constant state, simply because the condensate state is unique, and the system is invariant under translations. Therefore, the condensate state must be invariant under translations, and so must be the constant state

$$\varphi_0 = \frac{1}{\sqrt{V}}. \quad (3.32)$$

To compute the average number of particles in the condensate state, we project the wavefunction onto the condensate state: let

$$P_i := \mathbb{1}^{\otimes(i-1)} \otimes |\varphi_0\rangle\langle\varphi_0| \otimes \mathbb{1}^{\otimes(N-i)} \quad (3.33)$$

be the projector onto the subspace where the i -th particle is in the constant state (we use the “bra-ket” notation of quantum mechanics: $|\varphi_0\rangle\langle\varphi_0|f \equiv \langle\varphi_0, f\rangle\varphi_0$). The average number of particles in the condensate is then

$$\sum_{i=1}^N \langle\psi_0| P_i |\psi_0\rangle. \quad (3.34)$$

The condensate fraction is then

$$\eta_0 := \lim_{\substack{N, V \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{1}{N} \sum_{i=1}^N \langle\psi_0| P_i |\psi_0\rangle. \quad (3.35)$$

The Lee-Huang-Yang prediction of the condensation fraction for low densities is the following.

Conjecture 3.3

([LHY57, (41)])

For any potential $v \in L_1(\mathbb{R}^3)$ with $v \geq 0$ (actually, the potential may includes a hard-core component), as $\rho \rightarrow 0$,

$$1 - \eta_0 \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}} \quad (3.36)$$

where a is the scattering length of the potential.

In particular, this conjecture would imply Bose-Einstein condensation, which means that

$$\eta_0 > 0. \quad (3.37)$$

The two-point correlation function is the joint probability (in the usual quantum mechanical probability distribution $|\psi|^2$ of finding a particle at y and another at y' :

$$C_2(y - y') := \lim_{\substack{N, V \rightarrow \infty \\ \frac{N}{V} = \rho}} \sum_{i,j=1}^N \langle \psi_0 | \delta(x_i - y) \delta(x_j - y') | \psi_0 \rangle. \quad (3.38)$$

Lee, Huang and Yang made the following prediction.

Conjecture 3.4

([LHY57, (48)])

For any potential $v \in L_1(\mathbb{R}^3)$ with $v \geq 0$ (actually, the potential may includes a hard-core component), as $\sqrt{\rho a}|x| \rightarrow \infty$,

$$\frac{1}{\rho^2} C_2(x) - 1 \sim \frac{16\rho a^3}{\pi^3 (\sqrt{\rho a}|x|)^4} \quad (3.39)$$

where a is the scattering length of the potential.

Of these three conjectures, the only one that has been proved is Conjecture 3.2, and even so, the proof does not apply to all interactions v . The first order term, $2\pi\rho a/m$ was proved by Lieb and Yngvason [LY98], and the second order term was proved for potentials that are L_1 and L_3 by [FS20, FS23] and [YY09, BCS21]. [FS20] proved that (3.30) holds as an upper bound for soft-core potentials of finite range, and extended their result to hard core potentials in [FS23]. [YY09] proved the corresponding upper bound for small potentials, which was generalized to L_3 finite-range potentials by [BCS21]. The other two conjectures are still wide open. In particular, there is still no proof of Bose-Einstein condensation for interacting models.

3.4. Overview of the Simplified Approach

The Simplified Approach is what its name suggests: a simplified way of studying the interacting Bose gas that is considerably simpler than dealing with the Hamiltonian (3.1). By using the term “simplified”, we mean to imply that the results found using the approach are not (at least not yet) proven to be valid for the original Hamiltonian (3.1). In other words, it has (so far) not been used to prove any properties of (3.1) (though there is ongoing work in that direction). However, we have ample numerical and analytical evidence that the Simplified Approach captures a lot of the physics of the Bose gas. In fact, it captures significantly more than Bogolyubov

theory, which is also an approximate approach. This makes it quite an intriguing theory, and seems to be worth studying in more detail. We will define the Simplified Approach in the next section; for now, let us discuss the results predicted by Simplified Approach, to motivate the more detailed study of it that will follow.

The Simplified approach reduces the computation of the ground state energy to solving partial differential equations on \mathbb{R}^3 which is non-linear and non-local. “Equations” plural, because the Simplified Approach actually provides a family of equations that are more or less accurate and, correspondingly, harder or easier to study. Here we will discuss three of these equations, called the Big (3.59), Medium (3.67) and Simple (3.65) Equations. Solving these equations is not easy, but it is much more approachable than solving the equation (3.28), which involves an infinite number of particles, whereas the Simplified Approach provides single-particle equations.

Within the Simplified approach, we have proved Conjectures 3.2 [CJL20], 3.3 [CJL21] and 3.4 [Ja22]. In particular, we have proved that Bose-Einstein condensation occurs in the Simplified Approach. Thus, the Simplified Approach tells us at least as much as Bogolyubov theory (at least for the ground state of (3.1): it does not have anything to say about the thermal state (at least for now)). It goes quite a bit further. The large density expansion of the ground state energy per particle has long been computed for the Bose gas, at least in the case in which the Fourier transform of the potential is non-negative: $\hat{v} \geq 0$:

$$e_0 \sim_{\rho \rightarrow \infty} \frac{\rho}{2} \int dx v(x). \tag{3.40}$$

Within the Simplified Approach, this also holds. This is where things get significant: the Simplified Approach gives accurate results for *both low and high densities*. This is rather unusual: there are many effective theories in physics (Bogolyubov theory is one of them), but in almost all such cases, the effective theory works in just one parameter regime. The Simplified Approach works in two opposite regimes.

A natural question that arises is: if the Simplified Approach is accurate for small and large densities, how well does it do for intermediate densities? The energy per particle is plotted in Figure 3.1. The red crosses come from a Quantum Monte Carlo computation, which is the gold standard for quantum mechanical predictions (even though the theoretical control over the accuracy of this method is relatively incomplete; quantum mechanics is hard...). The gray dotted line is the Bogolyubov prediction, which we see is good for small densities, but quickly falls off the mark. The predictions for the Big, Medium and Simple Equations are plotted as well. The Simple Equation is accurate at small and large densities, as was mentioned above, but not great at intermediate densities. The Medium and Big Equations are quite accurate at *all* densities, especially the Big Equation which visually looks like a fit of the Quantum Monte Carlo data. This means that the Big Equation is capturing at least some of the physics of the many-body Bose gas *at all densities!* In addition, the Big Equation has a distinct advantage over Quantum Monte Carlo: it is much easier to solve numerically. Quantum Monte Carlo requires a significant amount of artistry: it is too costly to simulate very many particles, so the results need to be inferred from computations with a few dozen particles at most. On the other hand, the Big Equation is a partial differential equation that can be solved numerically with any of the usual tools.

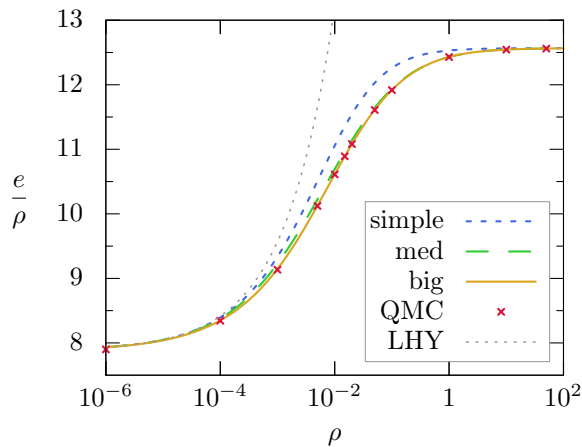


fig 3.1: [CHe21, Fig 1] The predictions of the energy per particle as a function of the density for the **Simple Equation**, **Medium Equation**, and **Big Equation**, compared to a **Quantum Monte Carlo** (QMC) simulation and the Lee-Huang-Yang (LHY) formula.

The condensate fraction is plotted in Figure 3.2. Again, we see that the Bogolyubov prediction is good for very small densities, but quickly goes wrong. The Big and Medium equations, on the other hand, seem to be very accurate throughout the range of densities.

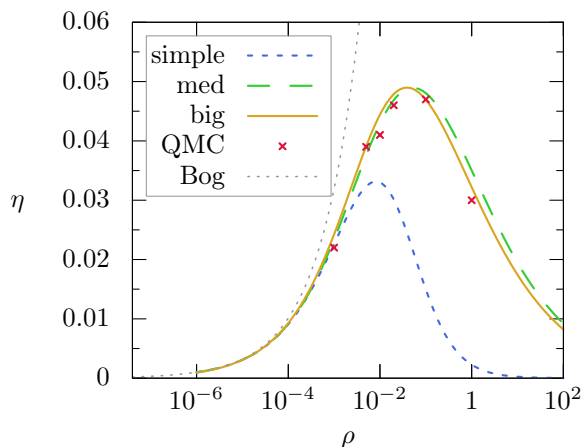


fig 3.2: [CHe21, Fig 3] The predictions of the condensate fraction as a function of the density for the **Simple Equation**, **Medium Equation**, and **Big Equation**, compared to a **Quantum Monte Carlo** (QMC) simulation and the Bogolyubov prediction (Bog).

Thus, the Simplified Approach provides us with a simple tool to study systems of interacting Bosons. The simplest equations can be studied analytically, and reproduce known and conjectured results [CJL20, CJL21, Ja22]. The more complicated equations are surprisingly accurate, while being much simpler to handle than traditional methods [CHe21, Ja23]. In particular, the Big Equation has been used [Ja23] to find evidence for a previously undiscovered phase in Bosons at intermediate densities.

3.5. The Simplified Approach and its approximations

The Simplified Approach dates back to a paper by Lieb from 1963 [Li63]. The discussion below follows [Li63] closely (though with more detail). The starting point of the Simplified

Approach is (3.28), which we write out using (3.1):

$$-\sum_{i=1}^N \frac{1}{2m} \Delta_i \psi_0 + \sum_{1 \leq i < j \leq N} v(x_i - x_j) \psi_0 = E_0 \psi_0. \quad (3.41)$$

3.5.1. Expression of the energy

In quantum mechanics, the probability distribution of the positions of the particles is $|\psi_0|^2$, so a natural approach to computing the energy from (3.41) would be to multiply both sides by ψ_0^* and integrate. This approach would lead to an expression of the energy as a functional to be minimized. However, this is quite difficult (if not impossible) to do when there are so many particles. Instead, we will simply integrate both sides of the equation (which is equivalent to taking a scalar product on both sides by the constant function (which, we recall, is the condensate wavefunction)). In doing so, we find the integral of the Laplacian of ψ_0 , which, since we took periodic boundary condition, is identically zero. We are then left with

$$\sum_{1 \leq i < j \leq N} \int dx_1 \cdots dx_N v(x_i - x_j) \psi_0(x_1, \dots, x_N) = E_0 \int dx_1 \cdots dx_N \psi_0(x_1, \dots, x_N) \quad (3.42)$$

which we can rewrite using the symmetry under particle exchanges as

$$E_0 = \frac{N(N-1)}{2V^2} \int dx_1 dx_2 v(x_1 - x_2) \frac{\int \frac{dx_3}{V} \cdots \frac{dx_N}{V} \psi_0(x_1, \dots, x_N)}{\int \frac{dy_1}{V} \cdots \frac{dy_N}{V} \psi_0(y_1, \dots, y_N)}. \quad (3.43)$$

This is written rather suggestively: if $\psi_0 / \int \psi_0$ were a probability distribution, then

$$g_2(x_1 - x_2) := \frac{\int \frac{dx_3}{V} \cdots \frac{dx_N}{V} \psi_0(x_1, \dots, x_N)}{\int \frac{dy_1}{V} \cdots \frac{dy_N}{V} \psi_0(y_1, \dots, y_N)} \quad (3.44)$$

would be its *two-point correlation function* (which is different from the quantum mechanical two-point correlation function in (3.38)). But, $\psi_0 / \int \psi_0$ is a probability distribution: by an argument based on the Perron-Frobenius theorem, see Exercise E5, $\psi_0 \geq 0$. Thus, we can rewrite E_0 in terms of the two-point correlation function g_2 :

$$\frac{E_0}{N} = \frac{(N-1)}{2V} \int dx v(x) g_2(x). \quad (3.45)$$

3.5.2. Hierarchy of equations

To compute g_2 , we follow the same idea, except that instead of integrating (3.41) with respect to all variables, we do so with respect to all but the first two: $\int dx_3 \cdots dx_N$:

$$\begin{aligned} & -\frac{1}{2m} \int dx_3 \cdots dx_N (\Delta_1 \psi_0 + \Delta_2 \psi_0) + v(x_1 - x_2) \int dx_3 \cdots dx_N \psi_0 + \\ & + \sum_{i=3}^{\infty} \int dx_3 \cdots dx_N (v(x_1 - x_i) + v(x_2 - x_i)) \psi_0 + \sum_{3 \leq i < j \leq N} \int dx_3 \cdots dx_N v(x_i - x_j) \psi_0 = \\ & = E_0 \int dx_3 \cdots dx_N \psi_0 \end{aligned} \quad (3.46)$$

which, again using the invariance under particle exchanges, reads

$$\begin{aligned} & -\frac{1}{2m} \int dx_3 \cdots dx_N (\Delta_1 \psi_0 + \Delta_2 \psi_0) + v(x_1 - x_2) \int dx_3 \cdots dx_N \psi_0 + \\ & + (N-2) \int dx_3 (v(x_1 - x_3) + v(x_2 - x_3)) \int dx_4 \cdots dx_N \psi_0 + \\ & + \frac{(N-2)(N-3)}{2} \int dx_3 dx_4 v(x_3 - x_4) \int dx_5 \cdots dx_N \psi_0 = E_0 \int dx_3 \cdots dx_N \psi_0. \end{aligned} \quad (3.47)$$

Defining the n -point correlation function of $\psi_0/\int\psi_0$ as

$$g_n(x_1, \dots, x_n) := \frac{\int \frac{dx_{n+1}}{V} \dots \frac{dx_N}{V} \psi_0(x_1, \dots, x_N)}{\int \frac{dy_1}{V} \dots \frac{dy_N}{V} \psi_0(y_1, \dots, y_N)} \quad (3.48)$$

we have

$$\begin{aligned} & -\frac{1}{m}\Delta g_2(x_1 - x_2) + v(x_1 - x_2)g_2(x_1 - x_2) + \\ & + \frac{N-2}{V} \int dx_3 (v(x_1 - x_3) + v(x_2 - x_3))g_3(x_1, x_2, x_3) + \\ & + \frac{(N-2)(N-3)}{2V^2} \int dx_3 dx_4 v(x_3 - x_4)g_4(x_1, x_2, x_3, x_4) = E_0 g_2(x_1 - x_2). \end{aligned} \quad (3.49)$$

We have thus obtained an equation for g_2 that involves g_3 and g_4 . We could keep on going, and we would find a full hierarchy of equations involving all the g_n .

3.5.3. Main approximation of the Simplified Approach

So far, we have done nothing fishy, and solving this hierarchy is equivalent to solving the original eigenvalue problem (3.28). However, this would be too difficult. Instead, we will make an approximation, which consists in expression g_3 and g_4 in terms of g_2 . This will turn (3.49) into an equation for g_2 alone.

Assumption 3.5

(*The factorization assumption*)

For $i = 3, 4$,

$$g_i(x_1, \dots, x_i) = \prod_{1 \leq j < l \leq i} (1 - u_i(x_j - x_l)) \quad (3.50)$$

in which u_i is bounded independently of V and is uniformly integrable in V :

$$|u_i(x)| \leq \bar{u}_i(x), \quad \int dx \bar{u}_i(x) \leq c_i \quad (3.51)$$

with c_i independent of V .

In other words, g_3 and g_4 factorize exactly into a product of pair terms. Here, we use the term “assumption” because it leads to the Simplified approach. However, it is really an *approximation* rather than an assumption: this factorization will certainly not hold true exactly. At best, one might expect that the assumption holds approximately in the limit of small and large ρ , and for distant points, as numerical evidence suggests in the translation invariant case. In this course, we will not attempt a proof that this approximation is accurate, and instead explore its consequences. Suffice it to say that this approximation is one of *statistical independence* that is reminiscent of phenomena arising in statistical mechanics when the density is low, that is, when the interparticle distances are large. In the current state of the art, we do not have much in the way of an explanation for why this statistical independence should hold; instead, we have extensive evidence, both numerical [CHe21] and analytical [CJL20, CJL21], that this approximation leads to very accurate predictions.

In order to derive a relation between g_3 , g_4 and g_2 , we will enforce a condition that holds true for the real g_3, g_4 . By definition (3.48),

$$\int \frac{dx_n}{V} g_n(x_1, \dots, x_n) = g_{n-1}(x_1, \dots, x_{n-1}). \quad (3.52)$$

We will enforce that this condition holds in order to compute values for u_3 and u_4 : specifically,

$$\int \frac{dx}{V} g_2(x) = 1, \quad \int \frac{dx_3}{V} g_3(x_1, x_2, x_3) = g_2(x_1 - x_2), \quad \int \frac{dx_3}{V} \frac{dx_4}{V} g_4(x_1, x_2, x_3, x_4) = g_2(x_1 - x_2). \quad (3.53)$$

Note that it is impossible for Assumption (3.5) to hold under the constraint that

$$\int \frac{dx_4}{V} g_4(x_1, x_2, x_3, x_4) = g_3(x_1, x_2, x_3) \quad (3.54)$$

which is one reason why Assumption 3.5 cannot hold exactly. As we will now see, (3.28), Assumption 3.5 and (3.53) together fix a definite value for u_3 and u_4 .

Theorem 3.6

If g_3, g_4 satisfies Assumption 3.5, the eigenvalue equation (3.28) and (3.53), then

$$u(x) := 1 - g_2(x) \quad (3.55)$$

satisfies

$$-\frac{1}{m} \Delta u(x) = (1 - u(x))v(x) + (1 - u(x))(-2\rho K(x) + \rho^2 L(x)) \quad (3.56)$$

where

$$S(x) := v(x)(1 - u(x)), \quad K(x) := S * u(x), \quad f_1 * f_2(x) := \int dz f_1(x - z)f_2(z) \quad (3.57)$$

$$L(x) := S * u * u(x) - 2u * (u(u * S))(x) + \frac{1}{2} \int dz dt S(z - t)u(x - z)u(x - t)u(z)u(t). \quad (3.58)$$

This equation is called the *Complete Equation*.

The proof of this theorem is simple in principle, but somewhat lengthy, and is deferred to Appendix A3.

3.6. The Equations of the Simplified Approach

We have thus introduced the first, and most difficult equation of the Simplified Approach: the *Complete Equation*, see Theorem 3.6. However, this equation is rather difficult to deal with, both analytically and numerically. From a numerical point of view, it is costly to compute nested integrals: the method used to carry out the numerics is a Gaussian quadrature, in which each integral is replaced by a sum of N terms, and taking an integral in n variables requires N^n points. In practice, a quintuple integral is near the upper limit of what is computable quickly on ordinary hardware (as of this writing). Several tricks are at our disposal to reduce the number of variables: in the case of a convolution, the integral is three dimensional, but by changing to *two-center bipolar coordinates*, we can reduce it to a double integral. In addition, (3.56) has fewer integrations in Fourier space, in which convolutions become products and vice versa. These allow us to reduce the computation to a sextuple integral (for details, see the documentation of the `simplesolv` software package [JaSS]), which is still rather heavy to compute. However, the sextuple integral appears only in the last term in (3.58), and if this term is dropped, we are left with only double integrals. We thus define an equation obtained from the Complete Equation in which we drop the last term in (3.58), which we will call the “*Big Equation*”.

Definition 3.7

(*Big Equation*)

$$-\frac{1}{m} \Delta u(x) = (1 - u(x))v(x) + (1 - u(x))(-2\rho K_{\text{bigeq}}(x) + \rho^2 L_{\text{bigeq}}(x)) \quad (3.59)$$

$$K_{\text{big eq}} := u * S, \quad S(y) := (1 - u(y))v(y) \quad (3.60)$$

$$L_{\text{big eq}} := u * u * S - 2u * (u(u * S)). \quad (3.61)$$

In practice, we have found that the predictions of the Big Equation are extremely close to those of the Complete Equation.

Whereas the Big Equation is (somewhat) easily computable numerically (see the documentation of the `simplesolv` software package [JaSS]), it remains rather difficult to study analytically. To simplify the equation, we will make two approximations. First, we assume that $u(x) \ll 1$, which is expected in the limit $|x| \rightarrow \infty$. This allows us to approximate

$$(1 - u)(-2\rho K + \rho^2 L) \approx -2\rho K + \rho^2 L, \quad L \approx u * u * S. \quad (3.62)$$

Second, we will replace S by a Dirac delta function (while preserving its integral):

$$S(x) \approx \delta(x) \int dx S(x) \equiv \frac{2e}{\rho} \delta(x), \quad e := \frac{\rho}{2} \int dx S(x) \equiv \frac{\rho}{2} \int dx (1 - u(x))v(x). \quad (3.63)$$

(The notation e is not innocuous: it is the prediction of the Simple Equation for the ground state energy, see (3.45).) The (rough) idea behind this approximation is that, viewed from a large distance, S can be replaced by a δ function (as long as the behavior is dominated by scattering events, the details of the potential should not matter, just its scattering length). Using this second approximation, we get

$$K \approx \frac{2e}{\rho} u, \quad L \approx \frac{2e}{\rho} u * u \quad (3.64)$$

which leads us to define the “*Simple Equation*” as follows.

Definition 3.8

(Simple Equation of the Simplified Approach)

$$-\frac{1}{m} \Delta u(x) = (1 - u(x))v(x) - 4eu(x) + 2e\rho u * u(x) \quad (3.65)$$

$$e := \frac{\rho}{2} \int dx (1 - u(x))v(x). \quad (3.66)$$

Finally, we define an intermediate equation, which is simpler than the Big Equation to compute, but has fewer approximations than the Simple Equation. As we will see below, this “*Medium Equation*” agrees quantitatively rather well with the Big Equation and the Bose gas. To define the Medium Equation, we make the approximation in (3.62), but not (3.64).

Definition 3.9

(Medium Equation of the Simplified Approach)

$$-\frac{1}{m} \Delta u(x) = (1 - u(x))v(x) - 2\rho u * S(x) + \rho^2 u * u * S(x) \quad (3.67)$$

$$S(x) := (1 - u(x))v(x). \quad (3.68)$$

3.7. Existence and uniqueness of solutions of the Simple Equation

We have defined four equations in the Simplified approach. These have a rather unusual structure. They are all non-linear, and are also non-local, because of the convolutions. The first question that arises is whether these equations have solutions. As of this writing, we only have an existence result for the Simple Equation. This result holds in all dimensions.

Theorem 3.10

(*[CJL20, Theorems 1.1, 1.3]*)

If $v \in L_1(\mathbb{R}^d) \cap L_p(\mathbb{R}^d)$ for $p > \max\{\frac{d}{2}, 1\}$ and $v \geq 0$, then (3.65) has an integrable solution u satisfying $0 \leq u(x) \leq 1$.

The crucial idea of the proof is that the Simple Equation is much easier to solve if we change the point of view: instead of fixing ρ and computing e and u , we fix e and compute ρ and u . Doing so turns the term $-4eu$ into a linear term. Next, we write the Simple Equation as a fixed point equation, by defining

$$\left(-\frac{1}{m}\Delta + v + 4e\right)u_n = v + 2e\rho_{n-1}u_{n-1} * u_{n-1}, \quad u_0 := 0 \quad (3.69)$$

with

$$\rho_n := \frac{2e}{\int dx (1 - u_n(x))v(x)}. \quad (3.70)$$

We will then prove the convergence of the iteration using the monotone convergence theorem. But first, let us prove a simple useful lemma.

Lemma 3.11

If the solution of the simple equation exists in $L_1(\mathbb{R}^d)$, then

$$\int dx u(x) = \frac{1}{\rho} \quad (3.71)$$

Proof: We integrate both sides of the Simple equation (3.65):

$$0 = \frac{2e}{\rho} - 4e \int dx u(x) + 2e\rho \left(\int dx u(x)\right)^2 \quad (3.72)$$

which we solve:

$$\int dx u(x) = \frac{1}{\rho}. \quad (3.73)$$

□

Let us translate this to the language of functional analysis: let

$$K_e := \left(-\frac{1}{m}\Delta + v + 4e\right)^{-1} \quad (3.74)$$

which is an operator from the Sobolev space $W_{2,p}(\mathbb{R}^d)$ to $L_p(\mathbb{R}^d)$ (see Appendix A1.1). Indeed, if $f \in W_{2,p}(\mathbb{R}^d)$, then, by the Sobolev inequality, $f \in L_q(\mathbb{R}^d)$ with $\frac{1}{q} = \frac{1}{p} - \frac{2}{d}$ and, by the triangle and Hölder inequalities,

$$\left\| -\frac{1}{m}\Delta f + vf + 4ef \right\|_p \leq \frac{1}{m}\|\Delta f\|_p + 4e\|f\|_p + \|v\|_{\frac{d}{2}}\|f\|_q < \infty \quad (3.75)$$

so $(-\frac{1}{m}\Delta + v + 4e)$ maps L_2 to $W_{2,p}$ (this is where the condition that v be at least $L_{\frac{d}{2}}$ comes from). In terms of K_e ,

$$u_n = K_e(v + 2e\rho_{n-1}u_{n-1} * u_{n-1}). \quad (3.76)$$

Lemma 3.12

The operator K_e is positivity preserving, see Appendix A1.4.

Proof: This follows directly from Theorem A1.15, taking v to be $m(v + 4e)$ and the fact that $\text{spec}(-\Delta + m(x + 4e)) \geq 4em$. \square

Lemma 3.13

ρ_n and u_n are pointwise increasing in n and

$$\int dx u_n(x) \leq \frac{1}{2e} \int dx (1 - u_n(x))v(x) \equiv \frac{1}{\rho_n}. \quad (3.77)$$

Proof: We proceed by induction.

1 - We have

$$u_0 = 0, \quad \rho_0 = \frac{2e}{\int dx v(x)} \quad (3.78)$$

and

$$u_1 = K_e v, \quad \rho_1 = \frac{2e}{\int dx v(x) - \int dx v(x)K_e v(x)}. \quad (3.79)$$

By Lemma 3.12,

$$u_1 \geq 0 \equiv u_0, \quad \rho_1 \geq \frac{2e}{\int dx v(x)} \equiv \rho_0. \quad (3.80)$$

Finally, u_1 satisfies

$$-\frac{1}{m}\Delta u_1 + 4eu_1 + vu_1 = v \quad (3.81)$$

so, integrating both sides,

$$\int dx u_1(x) = \frac{1}{4e} \int dx v(x)(1 - u_1(x)) \leq \frac{1}{2e} \int dx v(x)(1 - u_1(x)). \quad (3.82)$$

2 - Suppose the lemma holds for $n \geq 1$. By Lemma 3.12 and the inductive hypothesis,

$$u_{n+1} = K_e v + 2e\rho_n K_e u_n * u_n \geq K_e v + 2e\rho_{n-1} K_e u_{n-1} * u_{n-1} \equiv u_n. \quad (3.83)$$

In addition,

$$\rho_{n+1} = \frac{2e}{\int dx v(x)(1 - u_{n+1}(x))} \geq \frac{2e}{\int dx v(x)(1 - u_n(x))} = \rho_n. \quad (3.84)$$

Finally,

$$-\frac{1}{m}\Delta u_{n+1} + 4eu_{n+1} + vu_{n+1} = v + 2e\rho_n u_n * u_n \quad (3.85)$$

so, integrating both sides,

$$\int dx u_{n+1}(x) = \frac{1}{4e} \int dx v(x)(1 - u_{n+1}(x)) + \frac{1}{2}\rho_n \left(\int dx u_n(x) \right)^2 \quad (3.86)$$

so

$$\int dx u_{n+1}(x) \leq \frac{1}{4e} \int dx v(x)(1 - u_{n+1}(x)) + \frac{1}{2}\rho_n \int dx u_n(x) \int dx u_{n+1}(x) \quad (3.87)$$

and, by the inductive hypothesis,

$$\int dx u_n(x) \leq \frac{1}{2e} \int dx (1 - u_n(x))v(x) = \frac{1}{\rho_n} \quad (3.88)$$

so

$$\int dx u_{n+1}(x) \leq \frac{1}{4e} \int dx v(x)(1 - u_{n+1}(x)) + \frac{1}{2} \int dx u_{n+1}(x) \quad (3.89)$$

which implies

$$\int dx u_{n+1}(x) \leq \frac{1}{2e} \int dx v(x)(1 - u_{n+1}(x)). \quad (3.90)$$

□

Lemma 3.14

For all n ,

$$0 \leq u_n(x) \leq 1. \quad (3.91)$$

Proof: We proceed by induction. The lemma is trivial for $n = 0$ since $u_0 = 0$.

1 - First, we prove that $u_{n+1} \geq 0$. We have

$$u_{n+1} = K_e(v + 2e\rho_n u_n * u_n) \quad (3.92)$$

so, by Lemma 3.12,

$$u_{n+1} \geq 0. \quad (3.93)$$

2 - We now turn to $u_{n+1} \leq 1$. We have

$$\frac{1}{m} \Delta u_{n+1} = v(u_{n+1} - 1) + 4eu_{n+1} - 2e\rho_n u_n * u_n. \quad (3.94)$$

By Young's inequality (Theorem A1.4),

$$|u_n * u_n| \leq \|u_n\|_1 \|u_n\|_\infty \leq \|u_n\|_1 \quad (3.95)$$

and, by Lemma 3.13, $\|u_n\|_1 \leq \frac{1}{\rho_n}$ so

$$\frac{1}{m} \Delta u_{n+1} \geq v(u_{n+1} - 1) + 4eu_{n+1} - 2e. \quad (3.96)$$

Let

$$A := \{x : u_{n+1}(x) > 1\}. \quad (3.97)$$

Suppose that $A \neq \emptyset$. For $x \in A$,

$$\frac{1}{m} \Delta u_{n+1} \geq 2e > 0 \quad (3.98)$$

Therefore, u_{n+1} is subharmonic on A (see Appendix A2). By Theorem A2.2 u_{n+1} achieves its maximum on the boundary of A , but, by definition, $u_{n+1} = 1$ on its boundary. Therefore, inside A ,

$$u_{n+1} \leq 1 \quad (3.99)$$

which is a contradiction. Therefore A is empty (note that A is an open set because u_{n+1} is continuous, by virtue of being in $W_{2,p}(\mathbb{R}^d)$) and so

$$u_{n+1} \leq 1. \quad (3.100)$$

□

Lemma 3.15

Let

$$u(x) := \lim_{n \rightarrow \infty} u_n(x), \quad \rho(e) := \lim_{n \rightarrow \infty} \rho_n. \quad (3.101)$$

Both limits exist, $u \in W_{2,p}(\mathbb{R}^d)$ and u solves the Simple equation (3.65).

Proof: The limit of u_n exist by Lemmas 3.13 and (3.14) and the monotone convergence theorem. Furthermore, by Lemma 3.13,

$$\rho_n \leq \frac{1}{\int dx u_n(x)} \leq \frac{1}{\int dx u_1(x)} \equiv \frac{1}{\int dx K_e v(x)} < \infty \quad (3.102)$$

so, by monotone convergence, ρ_n converges as well. In addition, by Lemma 3.13,

$$\int dx u(x) \leq \frac{1}{2e} \|v\|_1 \quad (3.103)$$

so $u \in L_1(\mathbb{R}^d)$, and so, by dominated convergence, u_n converges in $L_1(\mathbb{R}^d)$. Moreover, by Lemma-3.14,

$$\|u\|_p^p \leq \|u\|_1 \quad (3.104)$$

and since $u_n - u \leq 1$,

$$\|u_n - u\|_p^p \leq \|u_n - u\|_1 \quad (3.105)$$

so u_n converges in L_p as well. Now, by Young's inequality (Theorem A1.4),

$$\|u * u - u_n * u_n\|_p = \|(u + u_n) * (u - u_n)\|_p \leq (\|u\|_1 + \|u_n\|_1) \|u_n - u\|_p \quad (3.106)$$

and so

$$\|(v + 2e\rho_n u_n * u_n) - (v + 2e\rho u * u)\|_p \leq 2e\rho \|u_n * u_n - u * u\|_p + 2e\|u_n * u_n\|_p(\rho - \rho_n). \quad (3.107)$$

Thus, $v + 2e\rho_n u_n * u_n$ converges in L_p , so $K_e(v + 2e\rho_n u_n * u_n)$ converges in $W_{2,p}$. Therefore,

$$u = K_e(v + 2e\rho u * u) \quad (3.108)$$

so u satisfies the Simple Equation. □

We are almost there: we have proved the existence of the solution of the modified problem where e is fixed instead of ρ . To prove Theorem 3.10, we need to prove that $e \mapsto \rho(e)$ can be inverted locally.

Lemma 3.16

The map $e \mapsto \rho(e)$ is continuous, and $\rho(0) = 0$ and $\lim_{e \rightarrow \infty} \rho(e) = \infty$. Therefore $e \mapsto \rho(e)$ can be inverted locally.

Proof: The trick of the proof is to consider the sequences

$$a_n := \int dx u_n(x), \quad b_n := \frac{1}{\rho_n} \equiv \frac{1}{2e} \int dx (1 - u_n(x))v(x). \quad (3.109)$$

By dominated convergence and Lemma 3.11,

$$\lim_{n \rightarrow \infty} a_n = \int dx u(x) = \frac{1}{\rho}, \quad \lim_{n \rightarrow \infty} b_n = \frac{1}{\rho} \quad (3.110)$$

and since u_n is increasing,

$$a_n \leq \frac{1}{\rho} \leq b_n. \quad (3.111)$$

Now, by (3.86)

$$2a_{n+1} = b_{n+1} + \rho_n a_n^2 \quad (3.112)$$

and so, since $b_n = 1/\rho_n$,

$$2(a_{n+1} - a_n) - (b_{n+1} - b_n) = \rho_n (b_n - a_n)^2 \quad (3.113)$$

which we sum for $n = 1 \dots$:

$$\frac{1}{\rho} + b_1 - 2a_1 = \sum_{n=1}^{\infty} \rho_n (b_n - a_n)^2. \quad (3.114)$$

Now, by (3.82),

$$a_1 = \frac{1}{4e} \int dx v(x)(1 - u_1(x)) = \frac{1}{2} b_1 \quad (3.115)$$

so

$$\frac{1}{\rho} = \sum_{n=1}^{\infty} \rho_n (b_n - a_n)^2 \quad (3.116)$$

and since ρ_n is increasing,

$$\sum_{n=1}^{\infty} (b_n - a_n)^2 \leq \frac{1}{\rho_1^2} = \left(\frac{1}{2e} \int dx (1 - K_e v(x)) v(x) \right)^2 \leq \left(\frac{1}{2e} \int dx v(x) \right)^2 \quad (3.117)$$

which is bounded uniformly in e on any compact interval $e \in [e_1, e_2]$. Thus, $b_n - a_n \rightarrow 0$ uniformly in e on any compact interval and thus ρ_n converges uniformly on $[e_1, e_2]$ so ρ is continuous on $[e_1, e_2]$. Since e_1, e_2 can be chosen arbitrarily, this holds for all e .

Finally,

$$\rho_n(0) = 0 \quad (3.118)$$

so $\rho(0) = 0$, and

$$\lim_{e \rightarrow \infty} \rho(e) = \infty \quad (3.119)$$

so, since ρ_n converges uniformly on all compacts,

$$\lim_{e \rightarrow \infty} \rho(e) = \infty. \quad (3.120)$$

□

This proves Theorem 3.10, and thus establishes the existence of a solution to the Simple Equation. But what of the uniqueness?

Theorem 3.17

(Uniqueness)

For any fixed e , the solution (u, ρ) to the Simple Equation with $u \in L_1(\mathbb{R}^d)$ and $u(x) \in [0, 1]$ is unique.

Proof: Consider two solutions (u, ρ) and (u', ρ') with $u'(x) \in [0, 1]$. We first show that $u' \geq u_n$ by induction. It is trivial at $n = 0$, and for $n \geq 1$,

$$u' - u_n = 2eK_e(\rho'u' * u' - \mathbb{1}_{n>1}\rho_{n-1}u_{n-1} * u_{n-1}) \quad (3.121)$$

where $\mathbb{1}_{n>1}$ is equal to 1 if $n > 1$ and 0 otherwise. Since

$$\rho' = \frac{2e}{\int dx (1 - u'(x))v(x)} \quad (3.122)$$

we have

$$\rho' \geq \frac{2e}{\int dx (1 - u_{n-1}(x))v(x)} \equiv \rho_{n-1} \quad (3.123)$$

so

$$\rho'u' * u' \geq \rho_{n-1}u_{n-1} * u_{n-1} \quad (3.124)$$

and

$$u' \geq u_n. \quad (3.125)$$

Thus

$$u' \geq u. \quad (3.126)$$

However, by Lemma 3.11,

$$\int dx u'(x) = \int dx u(x) = \frac{1}{\rho} \quad (3.127)$$

so

$$u = u'. \quad (3.128)$$

□

Thus, taking the point of view in which the energy e is fixed and ρ is computed as a function of e , the solution is unique. However, this does not imply that the solution to the problem in which ρ is fixed is unique: the mapping $e \mapsto \rho(e)$ may not be injective (it is surjective by Lemma 3.16). To prove that it is injective, one could prove that ρ is an increasing function of e (physically, it should be: the higher the density is, the higher the energy should be because the potential is repulsive). This has been proved for small and large values of e [CJL21], but, in general, it is still an open problem.

3.8. Energy of the Simple Equation

The Simplified Approach provides a natural prediction for the ground state energy per-particle (see (3.45)):

$$e = \frac{\rho}{2} \int dx (1 - u(x))v(x). \quad (3.129)$$

We have already seen numerical evidence for the fact that the Big and Medium equations provide very accurate predictions for the energy, see Figure 3.1. Let us now discuss an analytical result, which we can prove for the Simple Equation.

As was explained in Section 3.3, the ground state energy of the Bose gas has been computed at low and high densities, see (3.30) and (3.40). We have proved that both of these asymptotic expansions hold for the prediction of the Simple Equation.

Theorem 3.18

([CJL20, Theorem 1.4])

For the Simple Equation, under the assumptions of Theorem 3.10 for $d = 3$, as $\rho \rightarrow 0$,

$$e = \frac{2\pi}{m}\rho a \left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho}) \right) \quad (3.130)$$

where a is the scattering length of the potential, and as $\rho \rightarrow \infty$

$$e \sim_{\rho \rightarrow \infty} \frac{\rho}{2} \int dx v(x). \quad (3.131)$$

It is rather striking that the Simple Equation agrees with the Bose gas *both* at high and low densities. Note, however, that whereas (3.40) holds only for potentials of positive type (that is the Fourier transform of the potential \hat{v} is non-negative), (3.131) holds regardless of the sign of \hat{v} . The asymptotic agreement at high densities therefore only holds for positive type potentials.

Proof:

1 - Let us first prove (3.131), which is easier. By (3.66), it suffices to prove that

$$\lim_{\rho \rightarrow \infty} \int dx u(x)v(x) = 0. \quad (3.132)$$

Let

$$\chi_a := \{x : v(x) \geq a\} \quad (3.133)$$

and decompose

$$\int dx u(x)v(x) = \int_{\chi_a} dx u(x)v(x) + \int_{\mathbb{R}^d \setminus \chi_a} dx u(x)v(x) \quad (3.134)$$

which, by Lemmas 3.11 and 3.14, is bounded by

$$\int dx u(x)v(x) \leq \int_{\chi_a} dx v(x) + \frac{a}{\rho}. \quad (3.135)$$

Since v is integrable, $\int_{\chi_a} dx v(x) \rightarrow 0$ as $a \rightarrow \infty$. Therefore, taking $a = \sqrt{\rho}$,

$$\int_{\chi_a} v(x) dx + \frac{a}{\rho} \xrightarrow{\rho \rightarrow \infty} 0. \quad (3.136)$$

This proves (3.131).

2 - Let us now turn to (3.130). The scheme of the proof is as follows. We first approximate the solution u by w , which is defined as the decaying solution of

$$-\frac{1}{m} \Delta w(x) = (1 - u(x))v(x). \quad (3.137)$$

The energy of w is defined to be

$$e_w := \frac{\rho}{2} \int (1 - w(x))v(x) dx \quad (3.138)$$

and, as we will show, it is *close* to e , more precisely,

$$e - e_w = \frac{16\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2} \int dx v(x) + o(\rho^{\frac{3}{2}}). \quad (3.139)$$

In addition, (3.137) is quite similar to the scattering equation (3.6). In fact we will show that e_w is *close* to the energy $2\pi\rho a/m$ of the scattering equation

$$e_w - \frac{2\pi}{m}\rho a = -\frac{16\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2} \int dx \varphi(x)v(x) + o(\rho^{\frac{3}{2}}). \quad (3.140)$$

Summing (3.139) and (3.140), we find

$$e = \frac{2\pi}{m} \rho a \left(1 + \frac{32\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2\rho} + o(\sqrt{\rho}) \right), \quad (3.141)$$

from which (3.130) follows. We are thus left with proving (3.139) and (3.140).

2-1 - Proof of (3.139). By (3.66) and (3.138),

$$e - e_w = \frac{\rho}{2} \int dx (w(x) - u(x))v(x). \quad (3.142)$$

We will work in Fourier space

$$\hat{u}(k) := \int dx e^{ikx} u(x) \quad (3.143)$$

which satisfies, by (3.65),

$$\left(\frac{1}{m}k^2 + 4e \right) \hat{u}(k) = \hat{S}(k) + 2e\rho\hat{u}^2(k) \quad (3.144)$$

with

$$\hat{S}(k) := \int dx e^{ikx} (1 - u(x))v(x). \quad (3.145)$$

Therefore,

$$\hat{u}(k) = \frac{1}{\rho} \left(\frac{k^2}{4me} + 1 - \sqrt{\left(\frac{k^2}{4me} + 1 \right)^2 - \frac{\rho}{2e} \hat{S}(k)} \right). \quad (3.146)$$

Similarly, the Fourier transform of w is

$$\hat{w}(k) := \int dx e^{ikx} w(x) = \frac{m\hat{S}(k)}{k^2}. \quad (3.147)$$

Note that, as $|k| \rightarrow \infty$, $\hat{u} \sim \frac{m\hat{S}(k)}{k^2}$, so, while \hat{u} is not integrable, $\hat{u} - \hat{w}$ is. We invert the Fourier transform:

$$u(x) - w(x) = \frac{1}{8\pi^3\rho} \int dk e^{-ikx} \left(\frac{k^2}{4me} + 1 - \sqrt{\left(\frac{k^2}{4me} + 1 \right)^2 - \frac{\rho}{2e} \hat{S}(k) - \frac{m\rho\hat{S}(k)}{k^2}} \right). \quad (3.148)$$

We change variables to $\tilde{k} := \frac{k}{2\sqrt{me}}$:

$$u(x) - w(x) = \frac{(me)^{\frac{3}{2}}}{\rho\pi^3} \int d\tilde{k} e^{-i2\sqrt{me}\tilde{k}x} \left(\tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - \frac{\rho}{2e} \hat{S}(2\tilde{k}\sqrt{me}) - \frac{\rho}{2e} \frac{\hat{S}(2\tilde{k}\sqrt{me})}{2\tilde{k}^2}} \right). \quad (3.149)$$

Furthermore,

$$s \mapsto \left| \tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - s} - \frac{s}{2\tilde{k}^2} \right| \quad (3.150)$$

is monotone increasing. In addition, by (3.145) and (3.65), and using the fact that $u(x) \leq 1$ (see Lemma 3.14) and $v(x) \geq 0$,

$$|\hat{S}(k)| \leq \int dx |(1 - u(x))v(x)| = \frac{2e}{\rho}. \quad (3.151)$$

Therefore

$$\left| \tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - \frac{\rho}{2e} \hat{S}(2\tilde{k}\sqrt{me}) - \frac{\rho}{2e} \frac{\hat{S}(2\tilde{k}\sqrt{me})}{2\tilde{k}^2}} \right| \leq \left| \tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - 1} - \frac{1}{2\tilde{k}^2} \right|. \quad (3.152)$$

Therefore,

$$|u(x) - w(x)| \leq \frac{(me)^{\frac{3}{2}}}{\rho\pi^3} \int d\tilde{k} \left| \tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - 1} - \frac{1}{2\tilde{k}^2} \right| = \frac{32\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2\rho}. \quad (3.153)$$

By dominated convergence, and using the fact that $\hat{S}(0) = \frac{2e}{\rho}$,

$$\begin{aligned} \lim_{e \rightarrow 0} \frac{1}{(me)^{\frac{3}{2}}}(e - e_w) &= -\lim_{e \rightarrow 0} \frac{\rho}{2(me)^{\frac{3}{2}}} \int dx (u(x) - w(x))v(x) \\ &= -\frac{1}{2} \int dx v(x) \left(\frac{1}{\pi^3} \int \left(\tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - 1} - \frac{1}{2\tilde{k}^2} \right) d\tilde{k} \right) = \frac{16\sqrt{2}}{15\pi^2} \int dx v(x). \end{aligned} \quad (3.154)$$

Finally, since $u(x) \geq 0$,

$$e \leq \frac{\rho}{2} \int dx v(x) \quad (3.155)$$

so $e = O(\rho)$, and $e^{\frac{3}{2}} = O(\rho^{\frac{3}{2}})$. This proves (3.139). Incidentally, again by dominated convergence,

$$u(x) - w(x) = \frac{(me)^{\frac{3}{2}}}{\rho\pi^3} \int \left(\tilde{k}^2 + 1 - \sqrt{(\tilde{k}^2 + 1)^2 - 1} - \frac{1}{2\tilde{k}^2} \right) d\tilde{k} = -\frac{32\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2\rho} + \sqrt{\rho}f_\rho(x) \quad (3.156)$$

with

$$0 \leq f_\rho(x) \leq \frac{32\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2\rho}, \quad f_\rho(x) \xrightarrow{\rho \rightarrow 0} 0 \quad (3.157)$$

pointwise in x .

2-2 - Proof of (3.140). Let

$$\xi(r) := w(r) - \varphi(r). \quad (3.158)$$

By (3.137), (3.6) and (3.65),

$$(-\Delta + v(x))\xi(x) = -(u(x) - w(x))v(x). \quad (3.159)$$

Therefore, by Lemma 3.1,

$$e_w - \frac{2\pi}{m}\rho a = -\frac{\rho}{2} \int dx \xi(x)v(x) = -\frac{\rho}{2} \int dx v(x)(-\Delta + v)^{-1}((u - w)v)(x) \quad (3.160)$$

and

$$(-\Delta + v)^{-1}v(x) = \varphi(x) \quad (3.161)$$

so

$$e_w - \frac{2\pi}{m}\rho a = -\frac{\rho}{2} \int dx \varphi(x)(u(x) - w(x))v(x). \quad (3.162)$$

By (3.156),

$$e_w - \frac{2\pi}{m}\rho a = \frac{16\sqrt{2}(me)^{\frac{3}{2}}}{15\pi^2} \int dx \varphi(x)v(x) - \frac{\rho^{\frac{3}{2}}}{2} \int dx \varphi(x)f_\rho(x)v(x). \quad (3.163)$$

Since $x \mapsto f_\rho(x)$ is bounded, we can use dominated convergence to show (3.140). \square

3.9. Condensate fraction

The computation of the condensate fraction is not as straightforward as the energy. In fact, the Simplified Approach really only gives a clear prediction for the energy, through (3.45) which translates into (3.66). How do we compute the condensate fraction without knowing the expression of the wavefunction? The idea is to rewrite the condensate fraction in terms of the ground-state energy of an effective Hamiltonian. This is done in detail in Exercise E7. Proceeding in this way, we get a prediction for the condensate fraction. As was shown in Figure 3.2, the prediction of the Big and Medium equations are rather accurate for all densities, as the energy was. For the Simple Equation, we can prove an asymptotic expansion for low densities.

Theorem 3.19

([CJL21, Theorem 1.6])

For the Simple Equation, if $(1 + |x|^4)v(x) \in L_1(\mathbb{R}^3) \cap L_2(\mathbb{R}^3)$ and $v \geq 0$, as $\rho \rightarrow 0$,

$$1 - \eta \sim \frac{8\sqrt{\rho a^3}}{3\sqrt{\pi}} \tag{3.164}$$

where a is the scattering length of the potential.

Thus the Simple Equation reproduces the same prediction (3.36) as Bogolyubov theory.

The proof of this theorem is a bit more involved than the computation of the energy, though it is similar in spirit. We refer interested readers to [CJL21] for details.

4. Open problems

The Simplified Approach is thus a powerful tool to study the ground state of systems of interacting Bosons. It reproduces the predictions of Bogolyubov theory, but goes far beyond: it is asymptotically correct at high densities, and very accurate at intermediate densities as well. This tool may open the door to new attempts at proving some of the important outstanding problems concerning the Bose gas.

There are two directions that could be investigated to make a rigorous connection between the Simplified Approach and the Bose gas. One is to control the error made in the factorization assumption (see Assumption 3.5). Another is to construct an approximation of the ground state wavefunction directly, for instance, in Bijl-Dingle-Jastrow form:

$$\psi(x_1, \dots, x_N) = \prod_{i < j} e^{-u(x_i - x_j)} \tag{4.1}$$

where u is the solution of one of the equations of the Simplified Approach. Using our analysis of the Simplified Approach, we may be able to prove that (4.1) is a good approximation of the ground state wavefunction.

There are several open problems about the Bose gas that may be addressed in this way. A relatively simple problem is to prove (3.30) for hard-core potentials. As of this writing, it has been shown that (3.30) holds as a lower bound [FS23] for the hard core, but the corresponding upper bound has yet to be proved for the hard core. Another more difficult problem would be to prove (3.36), which would prove Bose-Einstein condensation. This is much more of a long shot, but nothing of this kind has been tried with these tools.

In addition, there is a number of open problems on the analysis of the Simplified Approach. For instance, the uniqueness of the solution to the Simple Equation has not been proved. It has been reduced to the question of the monotonicity of $e \mapsto \rho(e)$ (which should certainly hold, but it is not so easy to prove it). Moreover, the existence of the solution to the Medium and Big Equations has not been established. The proof we gave for the Simple Equation does not generalize easily to the other equations, so new ideas need to be found.

Appendices

A1. Elements of functional analysis

In this appendix we gather a few useful definitions and results from functional analysis.

A1.1. L_p and Sobolev spaces

Definition A1.1

(L_p and Sobolev spaces)

For $p \geq 1$ and Ω a metric space, we define the L_p space:

$$L_p(\Omega) := \left\{ f : \Omega \rightarrow \mathbb{R}, \left(\int dx |f(x)|^p \right)^{\frac{1}{p}} < \infty \right\} \quad (\text{A1.1})$$

and the Sobolev space

$$W_{k,p}(\Omega) := \left\{ f \in C^k(\Omega) : \forall l \in \{0, \dots, k\}, \partial^l f \in L_p(\Omega) \right\} \quad (\text{A1.2})$$

in which $C^k(\Omega)$ is the set of k -times continuously differentiable functions on Ω .

Theorem A1.2

(Hölder's inequality [Te14, Problem 0.26])

If $f \in L_p(\Omega)$ and $g \in L_q(\Omega)$, then $fg \in L_r(\Omega)$ with

$$\frac{1}{r} = \frac{1}{p} + \frac{1}{q} \quad (\text{A1.3})$$

and

$$\|fg\|_r \leq \|f\|_p \|g\|_q. \quad (\text{A1.4})$$

Theorem A1.3

(Sobolev embedding theorem)

For $k, l \geq 0$ and $p, q \geq 1$, $d \geq 1$, such that

$$\frac{1}{p} - \frac{k}{d} = \frac{1}{q} - \frac{l}{d} \quad (\text{A1.5})$$

we have

$$W_{k,p}(\mathbb{R}^d) \subset W_{l,q}(\mathbb{R}^d). \quad (\text{A1.6})$$

In particular,

$$W_{k,p}(\mathbb{R}^d) \subset L_q(\mathbb{R}^d), \quad \frac{1}{q} = \frac{1}{p} - \frac{k}{d}. \quad (\text{A1.7})$$

Theorem A1.4

(Young's inequality)

If $f \in L_p(\Omega)$ and $g \in L_q(\Omega)$, then $f * g \in L_r(\Omega)$ with

$$1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q} \quad (\text{A1.8})$$

and

$$\|f * g\|_r \leq \|f\|_p \|g\|_q. \quad (\text{A1.9})$$

A1.2. The Trotter product formula

Theorem A1.5

(Trotter product formula [Te14, Theorem 5.11])

Given two operators A and B on a Hilbert space such that A , B and $A + B$ are self-adjoint, and bounded from below, then for $t \geq 0$,

$$e^{-t(A+B)} = \lim_{N \rightarrow \infty} \left(e^{-t\frac{1}{N}A} e^{-t\frac{1}{N}B} \right)^N. \quad (\text{A1.10})$$

A1.3. Compact and trace-class operators

Definition A1.6

(Trace)

Given a separable Hilbert space with an orthonormal basis $\{\varphi_i\}_{i \in \mathbb{N}}$, the trace of an operator A is formally defined as

$$\text{Tr}(A) := \sum_{i=0}^{\infty} \langle \varphi_i | A | \varphi_i \rangle. \quad (\text{A1.11})$$

If this expression is finite, then A is said to be trace-class.

Definition A1.7

(Compact operators)

The set of compact operators on a Hilbert space is the closure of the set of finite-rank operators.

Theorem A1.8

([Te14, Theorem 6.6])

If A is a compact self-adjoint operator on a Hilbert space, then its spectrum consists of an at most countable set of eigenvalues.

Theorem A1.9

Trace class operators are compact.

Theorem A1.10

([Te14, Lemma 5.5])

If A is compact and B is bounded, then KA and AK are compact.

Theorem A1.11

Let Δ be the Laplacian on $L_2(\mathbb{R}^d / (L\mathbb{Z})^d)$ (the same result holds for Dirichlet and Neumann boundary conditions as well). For any function v on $[0, L]^d$ that is bounded below, $e^{t(-\Delta+v)}$ is compact for any $t \geq 0$.

Proof: First of all, $e^{-t\Delta}$ is trace class: using the basis e^{ikx} with $k \in (\frac{2\pi}{L}\mathbb{Z})^d$

$$\text{Tre}^{-t\Delta} = \sum_{k \in (\frac{2\pi}{L}\mathbb{Z})^d} e^{-tk^2} < \infty. \quad (\text{A1.12})$$

By Theorem A1.9, $e^{-t\Delta}$ is compact. By the Trotter product formula, Theorem A1.5,

$$e^{-t\Delta+tv} = \lim_{N \rightarrow \infty} (e^{-\frac{t}{N}\Delta} e^{\frac{t}{N}v})^N \quad (\text{A1.13})$$

and by Theorem A1.10, $(e^{-\frac{t}{N}\Delta} e^{\frac{t}{N}v})^N$ is compact. Since the set of compact operators is closed, so is $e^{t(-\Delta+v)}$. \square

A1.4. Positivity preserving operators

Definition A1.12

(Positivity preserving operators)

An operator A from a Banach space of real-valued functions \mathcal{B}_1 to another \mathcal{B}_2 is said to be *positivity preserving* if, for any $f \in \mathcal{B}_1$ such that $f(x) \geq 0$, $Af(x) \geq 0$.

Lemma A1.13

If $\text{spec}(A+B) > \epsilon > 0$, and e^{-tA} and e^{-tB} are positivity preserving for all $t > 0$, then for all $t > 0$, $e^{-t(A+B)}$ and $(A+B)^{-1}$ are positivity preserving.

Proof: We write

$$(A^{-1} + B)^{-1} = \int_0^\infty dt e^{-t(A^{-1}+B)} \quad (\text{A1.14})$$

indeed, by the spectral theorem,

$$\int_0^\infty dt e^{-t(A^{-1}+B)} = \int_0^\infty dt \int_{\text{spec}(A^{-1}+B)} d\sigma e^{-t\sigma} P_\sigma = \int_{\text{spec}(A^{-1}+B)} d\sigma \frac{1}{\sigma} P_\sigma = (A^{-1} + B)^{-1}. \quad (\text{A1.15})$$

By the Trotter product formula (Theorem A1.5),

$$e^{-t(A^{-1}+B)} = \lim_{N \rightarrow \infty} (e^{-\frac{t}{N}A^{-1}} e^{-\frac{t}{N}B})^N. \quad (\text{A1.16})$$

\square

Theorem A1.14

(Positivity of the heat kernel)

Given $t > 0$, the operator $e^{t\Delta}$ from $L_2(\mathbb{R}^d)$ to $L_2(\mathbb{R}^d)$ is positivity preserving.

Proof: If

$$\psi_t(x) = e^{t\Delta}\psi_0(x) \quad (\text{A1.17})$$

then

$$\partial_t \psi_t(x) = \Delta \psi_t(x). \quad (\text{A1.18})$$

The Fourier transform of ψ_t is defined as

$$\hat{\psi}_t(k) := \int dx e^{ikx} \psi_t(x) \quad (\text{A1.19})$$

which satisfies

$$\partial_t \hat{\psi}_t(k) = -k^2 \hat{\psi}_t(k) \quad (\text{A1.20})$$

so

$$\hat{\psi}_t(k) = e^{-tk^2} \hat{\psi}_0(k) \quad (\text{A1.21})$$

thus, taking an inverse Fourier transform,

$$\psi_t(x) = \left(\int \frac{dk}{(2\pi)^d} e^{-ikx} e^{-tk^2} \right) * \psi_0(x) \quad (\text{A1.22})$$

and

$$\int \frac{dk}{(2\pi)^d} e^{-ikx} e^{-tk^2} = \prod_{i=1}^d \int_{-\infty}^{\infty} \frac{dk_i}{2\pi} e^{-ik_i x_i} e^{-tk_i^2} = \prod_{i=1}^d \frac{1}{2\sqrt{t\pi}} e^{-\frac{1}{4t}x_i^2} = \frac{1}{(4\pi t)^{\frac{d}{2}}} e^{-\frac{1}{4t}|x|^2} \geq 0. \quad (\text{A1.23})$$

□

Theorem A1.15

Given $t > 0$ and a function v , the operator $e^{-t(-\Delta+v)}$ is positivity preserving. In addition, if $\text{spec}(-\Delta + v) > \epsilon > 0$, then $(-\Delta + v)^{-1}$ is positivity preserving.

Proof: By the Trotter product formula (Theorem A1.5),

$$e^{-t(-\Delta+v)} = \lim_{N \rightarrow \infty} (e^{\frac{t}{N}\Delta} e^{-\frac{t}{N}v})^N \quad (\text{A1.24})$$

which is positivity preserving, because $e^{-\frac{t}{N}v}$ is a multiplication operator by a non-negative function. The second point follows from lemma A1.13, in which we take $A = -\Delta$ and $B = v$ (e^{-tv} is a multiplication operator by a non-negative function, which is positivity preserving, and so is $e^{t\Delta}$, by Theorem A1.14). □

Remark: In particular, taking the potential to be $\eta + v(x)$, this implies that $e^{-t(-\Delta+v(x)+\eta)}$ and $(-\Delta + v(x) + \eta)^{-1}$ are positivity preserving for any $\eta, v(x) \geq 0$.

Lemma A1.16

If A is positivity preserving, $f \in L_1(\mathbb{R}^d)$ such that $f \geq 0$ and $\text{spec}(A - f*) > \epsilon > 0$ and e^{-tA} is positivity preserving, then $(A - f*)^{-1}$ is positivity preserving.

Proof: This follows from lemma A1.13, noting that e^{tf*} is obviously positivity preserving. □

Remark: In particular, if $v(x), \eta > 0$, $\|f\|_1 \leq \eta$, then $(-\Delta + v + \eta - f*)^{-1}$ is positivity preserving. The assumption $\|f\|_1 \leq \eta$ ensures that $-\Delta + v + \eta - f*$ has a spectrum that is bounded away from 0.

A1.5. The Perron-Frobenius theorem

Theorem A1.17

((Generalized) Perron-Frobenius theorem)

Let A be a compact operator from a Banach space of real-valued functions \mathcal{B}_1 to another \mathcal{B}_2 . If A is positivity preserving (see Definition A1.12) and has a finite and positive spectral radius $r(A)$ ($r(A) := \sup_{\lambda \in \text{spec}(A)} |\lambda|$), then $r(A)$ is a non-degenerate eigenvalue whose corresponding eigenvector f is non-negative:

$$Af = r(A)f, \quad f(x) \geq 0. \quad (\text{A1.25})$$

A2. Elements of harmonic analysis

In this appendix, we state some useful results from harmonic analysis.

Definition A2.1

(*Harmonic, subharmonic and superharmonic functions*)

A function $f \in C^2(\mathbb{R}^d)$ is said to be *harmonic* on $A \subset \mathbb{R}^d$ if $\forall x \in A$,

$$\Delta f(x) = 0 \tag{A2.1}$$

it is *subharmonic* if

$$\Delta f(x) \geq 0 \tag{A2.2}$$

and *superharmonic* if

$$\Delta f(x) \leq 0. \tag{A2.3}$$

Theorem A2.2

(*[LL01, Theorem 9.4]*)

A function that is subharmonic on A achieves its maximum on the boundary of A . A function that is superharmonic on A achieves its minimum on the boundary of A .

A3. Proof of Theorem 3.6

A3.1. Factorization

We will first compute u_3, u_4 . We need to compute these up to order V^{-2} , because one of the terms in the equation is of order V (see below).

A3.1.1. Factorization of g_3

Lemma A3.1

Assumption 3.5 with $i = 3$ and (3.53) imply that

$$g_3(x, y, z) = (1 - u_3(x - y))(1 - u_3(x - z))(1 - u_3(y - z))(1 + O(V^{-2})) \tag{A3.1}$$

with

$$u_3(x - y) := u(x - y) + \frac{w_3(x - y)}{V} \tag{A3.2}$$

$$w_3(x - y) := (1 - u(x - y)) \int dz u(x - z)u(y - z). \tag{A3.3}$$

Proof: Using (3.53) in (3.50),

$$g_2(x_1 - x_2) = (1 - u_3(x_1 - x_2)) \int \frac{dx_3}{V} (1 - u_3(x_1 - x_3))(1 - u_3(x_2 - x_3)). \tag{A3.4}$$

1 - We first expand to order V^{-1} . By (3.51),

$$\int \frac{dz}{V} u_3(x - z) = O(V^{-1}) \tag{A3.5}$$

so,

$$g_2(x-y) \equiv 1 - u(x-y) = (1 - u_3(x-y))(1 + O(V^{-1})). \quad (\text{A3.6})$$

Therefore,

$$u_3(x-y) = u(x-y)(1 + O(V^{-1})). \quad (\text{A3.7})$$

2 - We push the expansion to order V^{-2} : (A3.4) is

$$g_2(x-y) = (1 - u_3(x-y)) \int \frac{dz}{V} (1 - u_3(x-z) - u_3(y-z) + u_3(x-z)u_3(y-z)). \quad (\text{A3.8})$$

By (A3.7),

$$(1 - u_3(x-y)) = (1 - u(x-y)) \cdot \left(1 + \int \frac{dz}{V} (u(x-z) + u(y-z) - u(x-z)u(y-z)) + O(V^{-2}) \right). \quad (\text{A3.9})$$

Furthermore, by (3.53),

$$\int \frac{dx}{V} (1 - u(x)) = 1 \quad (\text{A3.10})$$

so

$$\int dx u(x) = 0. \quad (\text{A3.11})$$

Thus,

$$1 - u_3(x-y) = (1 - u(x-y)) \left(1 - \int \frac{dz}{V} u(x-z)u(y-z) + O(V^{-2}) \right). \quad (\text{A3.12})$$

□

A3.1.2. Factorization of g_4

Lemma A3.2

Assumption 3.5 and (3.53) imply that

$$g_4(x_1, x_2, x_3, x_4) = \left(\prod_{i < j} (1 - u_4(x_i - x_j)) \right) (1 + O(V^{-2})) \quad (\text{A3.13})$$

with

$$u_4(x-y) := u(x-y) + \frac{2w_3(x-y)}{V} \quad (\text{A3.14})$$

where w_3 is the same as in Lemma A3.1.

Proof: Using (3.53) in (3.50),

$$g_2(x_1 - x_2) = (1 - u_4(x_1 - x_2)) \int \frac{dx_3 dx_4}{V^2} (1 - u_4(x_1 - x_3))(1 - u_4(x_1 - x_4)) \cdot (1 - u_4(x_2 - x_3))(1 - u_4(x_2 - x_4))(1 - u_4(x_3 - x_4)). \quad (\text{A3.15})$$

1 - We expand to order V^{-1} . By (3.51),

$$\int \frac{dz}{V} u_4(x-z) = O(V^{-1}) \quad (\text{A3.16})$$

so

$$g_2(x-y) \equiv 1 - u(x-y) = (1 - u_4(x-y))(1 + O(V^{-1})) \quad (\text{A3.17})$$

so

$$u_4(x-y) = u(x-y)(1 + O(V^{-1})). \quad (\text{A3.18})$$

2 - We push the expansion to order V^{-2} : by (3.51),

$$\int \frac{dzdt}{V^2} u_4(x-z)u_4(y-t) = O(V^{-2}), \quad \int \frac{dzdt}{V^2} u_4(x-z)u_4(z-t) = O(V^{-2}) \quad (\text{A3.19})$$

$$\int \frac{dzdt}{V^2} u_4(x-z)u_4(x-t) = O(V^{-2}) \quad (\text{A3.20})$$

so

$$1 - u(x-y) = (1 - u_4(x-y)) \cdot \left(1 + \int \frac{dzdt}{V^2} (-2u_4(x-z) - 2u_4(y-z) - u_4(z-t) + 2u_4(x-z)u_4(y-z)) + O(V^{-2}) \right). \quad (\text{A3.21})$$

By (A3.18),

$$1 - u_4(x-y) = (1 - u(x-y)) \cdot \left(1 + \int \frac{dzdt}{V^2} (2u(x-z) + 2u(y-z) + u(z-t) - 2u(x-z)u(y-z)) + O(V^{-2}) \right). \quad (\text{A3.22})$$

By (A3.11),

$$1 - u_4(x-y) = (1 - u(x-y)) \left(1 - 2 \int \frac{dz}{V} u(x-z)u(y-z) + O(V^{-2}) \right). \quad (\text{A3.23})$$

□

A3.2. Proof of Theorem 3.6

1 - First of all, by (3.45),

$$E_0 = \frac{N(N-1)}{2V} \int dx v(x)(1 - u(x)). \quad (\text{A3.24})$$

2 - We rewrite (3.49) using Lemmas, A3.1 and A3.2. Let

$$G_3 := \frac{N-2}{V} \int dx_3 (v(x_1 - x_3) + v(x_2 - x_3))g_3(x_1, x_2, x_3) \quad (\text{A3.25})$$

and

$$G_4 := \frac{(N-2)(N-3)}{2V^2} \int dx_3 dx_4 v(x_3 - x_4)g_4(x_1, x_2, x_3, x_4). \quad (\text{A3.26})$$

By Lemma A3.1,

$$G_3(x-y) = \frac{N}{V} (1 - u(x-y)) \cdot \left(\int dz (v(x-z) + v(y-z))(1 - u(x-z))(1 - u(y-z)) + O(V^{-1}) \right) \quad (\text{A3.27})$$

and by Lemma A3.2,

$$G_4(x-y) = \left(\frac{N^2}{2V^2}(1-u_4(x-y)) \int dzdt v(z-t)(1-u_4(z-t))\Pi(x,y,z,t) - \frac{5N}{2V^2}(1-u(x-y)) \int dzdt v(z-t)(1-u(z-t)) + O(V^{-1}) \right) \quad (\text{A3.28})$$

$$\Pi(x,y,z,t) := (1-u(x-z))(1-u(x-t))(1-u(y-z))(1-u(y-t)). \quad (\text{A3.29})$$

The first term in G_4 is of order V : by (A3.14),

$$\begin{aligned} & \frac{N^2}{2V^2}(1-u_4(x-y)) \int dzdt v(z-t)(1-u_4(z-t))\Pi(x-y-z-y) = \\ & = \frac{N^2}{2V^2}(1-u(x-y)) \int dzdt v(z-t)(1-u(z-t)) - \\ & - \frac{N^2}{V^3}w_3(x-y) \int dzdt v(z-t)(1-u(z-t)) - \\ & - \frac{N^2}{V^3}(1-u(x-y)) \int dzdt v(z-t)w_3(z-t) + \\ & + \frac{N^2}{2V^2}(1-u(x-y)) \int dzdt v(z-t)(1-u(z-t)) (\Pi(x,y,z,t) - 1) + O(V^{-1}) \end{aligned} \quad (\text{A3.30})$$

in which the only term of order V is the first one, and is equal to the term of order V in E_0g_2 :

$$(1-u(x-y)) \frac{N^2}{2V} \int dz v(z)(1-u(z)) \quad (\text{A3.31})$$

and thus cancels out. Therefore, recalling that $\rho = \frac{N}{V}$,

$$\left(-\frac{1}{m}\Delta + v(x-y) + \bar{G}_3(x-y) + \bar{G}_4(x-y) - \bar{E}_0 \right) (1-u(x-y)) = O(V^{-1}) \quad (\text{A3.32})$$

with

$$\bar{G}_3(x-y) := \rho \int dz (v(x-z) + v(y-z))(1-u(x-z))(1-u(y-z)) \quad (\text{A3.33})$$

and by (A3.3),

$$\begin{aligned} \bar{G}_4(x-y) := & -\frac{\rho}{2} \left(5 + 2\rho \int dr u(x-r)u(y-r) \right) \int \frac{dzdt}{V} v(z-t)(1-u(z-t)) - \\ & -\rho^2 \int \frac{dzdt}{V} v(z-t)(1-u(z-t)) \int dr u(z-r)u(t-r) + \\ & + \frac{\rho^2}{2} \int dzdt v(z-t)(1-u(z-t)) (\Pi(x,y,z,t) - 1) \end{aligned} \quad (\text{A3.34})$$

$$\bar{E}_0 = \frac{\rho}{2} \int \frac{dx dy}{V} v(x-y)(1-u(x-y)). \quad (\text{A3.35})$$

3 - Thus, in the thermodynamic limit, using translation invariance,

$$\bar{E}_0 = -\frac{\rho}{2} \int dz v(z)(1-u(z)). \quad (\text{A3.36})$$

Furthermore,

$$\bar{G}_3(x) = -4\bar{E}_0 - 2\rho u * S(x). \quad (\text{A3.37})$$

In addition,

$$-\frac{5\rho}{2} \int \frac{dzdt}{V} v(z-t)(1-u(z-t)) = 5\bar{E}_0 \quad (\text{A3.38})$$

$$-\rho^2 \int dr u(x-r)u(y-r) \int \frac{dzdt}{V} v(z-t)(1-u(z-t)) = 2\rho\bar{E}_0 u * u(x-y) \quad (\text{A3.39})$$

$$-\rho^2 \int \frac{dzdt}{V} v(z-t)(1-u(z-t)) \int dr u(z-r)u(t-r) = -\rho^2 \int dz S(z)u * u(z) \quad (\text{A3.40})$$

and, by (A3.11) and (A3.29),

$$\begin{aligned} & \frac{\rho^2}{2} \int dzdt v(z-t)(1-u(z-t))(\Pi(x,y,z,t) - 1) = \\ & = \rho^2 \left(\int dz S(z)u * u(z) - \frac{2}{\rho} u * u(x-y)\bar{E}_0 + u * u * S(x-y) \right. \\ & \quad \left. - 2u * (u(u * S))(x-y) + \frac{1}{2} \int dzdt u(y-z)u(y-t)u(x-z)u(x-t)S(z-t) \right). \end{aligned} \quad (\text{A3.41})$$

Inserting these into (A3.32), we find (3.56). \square

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Exercises

Exercise E1 (solution on p. 45)

Prove (2.24) starting from (2.23).

Exercise E2 (solution on p. 45)

Check (2.27) explicitly using the Riemann theorem. Prove that $\mu \mapsto \rho(\mu)$ is strictly increasing using the dominated convergence theorem. Prove (2.28) and (2.29).

Exercise E3 (solution on p. 45)

Compute the analogue of (2.24) for an ideal gas of *Fermions*:

$$\langle \mathcal{B}_q \rangle = \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} + 1} \quad (\text{E3.1})$$

Hint: Proceed in the same way as the ideal gas of Bosons by parametrizing the space using the occupation number of plane waves e^{ikx} . Except that now, because the wavefunctions are antisymmetric, there can only be 0 or 1 particle in each state, so the sums over N_k are over $\{0, 1\}$. Can there be Bose-Einstein condensation for the ideal gas of Fermions?

Exercise E4 (solution on p. 46)

Prove that the solution of (3.17) is (3.18).

Hint: use the fact that $\psi \rightarrow 1$ as $|x| \rightarrow \infty$, as well as the fact that ψ is continuous at 0 and at R .

Exercise E5 (solution on p. 46)

Prove that the ground state ψ_0 of (3.1) is unique and $\psi_0 \geq 0$.

Hint: Instead of the Hamiltonian H_N , consider the operator e^{-tH_N} for $t \geq 0$. Check that Theorem A1.15 applies, so that e^{-tH_N} is positivity preserving (see Definition A1.12). Use the Perron-Frobenius theorem (Theorem A1.17) to conclude.

Exercise E6 (solution on p. 46)

In this exercise, we will derive an alternate proof that $\psi_0 \geq 0$ under the extra assumption that v is continuous. To do so, consider the energy of ψ_0 :

$$\mathcal{E}(\psi_0) := \langle \psi_0 | H_N | \psi_0 \rangle = \int_{(\mathbb{R}/(L\mathbb{Z}))^{3N}} dx \left(-\frac{1}{2m} \psi_0^*(x) \Delta \psi_0(x) + V(x) |\psi_0(x)|^2 \right) \quad (\text{E6.1})$$

where Δ is the Laplacian on \mathbb{R}^{3N} and $V(x) \equiv \sum_{i < j} v(x_i - x_j)$. Prove that

$$\mathcal{E}(|\psi_0\rangle) = \mathcal{E}(\psi_0) \quad (\text{E6.2})$$

and use that to prove that $\psi_0 \geq 0$.

Exercise E7 (solution on p. 47)

In this exercise, we will show how to compute the condensate fraction in terms of the ground state energy of an effective Hamiltonian. Let

$$\tilde{H}_N(\epsilon) := H_N + \epsilon \sum_{i=1}^N P_i \quad (\text{E7.1})$$

where P_i is the projector onto the constant state (A3.29) (recall (3.35)). Let $\tilde{E}_0(\epsilon)$ denote the ground state energy of $\tilde{H}_N(\epsilon)$. Prove that

$$\eta_0 = \lim_{\substack{N, V \rightarrow \infty \\ \frac{N}{V} = \rho}} \frac{1}{N} \partial_\epsilon \tilde{E}_0 |_{\epsilon=0}. \quad (\text{E7.2})$$

Solution E1

To compute

$$\sum_{N=0}^{\infty} N e^{-tN} \quad (\text{SE1.1})$$

we differentiate

$$\sum_{N=0}^{\infty} e^{-tN} = \frac{1}{1 - e^{-t}} \quad (\text{SE1.2})$$

with respect to $-t$:

$$\sum_{N=0}^{\infty} N e^{-tN} = \frac{e^{-t}}{(1 - e^{-t})^2}. \quad (\text{SE1.3})$$

Therefore, by (2.22) and (2.23),

$$\langle \mathcal{B}_q \rangle = \frac{e^{-\beta(\frac{k^2}{2m} - \mu)}}{1 - e^{-\beta(\frac{k^2}{2m} - \mu)}} \frac{\prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{1 - e^{-\beta(\frac{k^2}{2m} - \mu)}}}{\prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{1 - e^{-\beta(\frac{k^2}{2m} - \mu)}}} = \frac{e^{-\beta(\frac{k^2}{2m} - \mu)}}{1 - e^{-\beta(\frac{k^2}{2m} - \mu)}} \quad (\text{SE1.4})$$

from which (2.24) follows.

Solution E2

1 - (2.26) is of the form

$$\rho_L(\mu) = \frac{1}{(2\pi)^3} \frac{1}{D} \sum_{k \in \mathbb{Z}^3} f(Dk) \quad (\text{SE2.1})$$

with

$$D \equiv \frac{L}{2\pi}, \quad f(k) := \frac{1}{e^{\beta(\frac{k^2}{2m} - \mu)} - 1} \quad (\text{SE2.2})$$

so (2.27) follows from the Riemann theorem.

2 - For $\mu < 0$,

$$\left| \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1} \right| \quad (\text{SE2.3})$$

is integrable and, for $\mu_0 < \mu < 0$,

$$\left| \partial_\mu \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1} \right| = \beta \frac{e^{\beta(\frac{q^2}{2m} - \mu)}}{(e^{\beta(\frac{q^2}{2m} - \mu)} - 1)^2} \leq \beta \frac{e^{\beta(\frac{q^2}{2m} - \mu_0)}}{(e^{\beta \frac{q^2}{2m}} - 1)^2}. \quad (\text{SE2.4})$$

Now, since

$$e^{\beta \frac{q^2}{2m}} - 1 \sim_{q \rightarrow 0} \frac{\beta q^2}{2m} \quad (\text{SE2.5})$$

this is integrable in dimensions three or more.

3 - Since

$$\left| \frac{1}{e^{\beta(\frac{q^2}{2m} - \mu)} - 1} \right| \leq \frac{1}{e^{\beta(\frac{q^2}{2m})} - 1} \quad (\text{SE2.6})$$

is integrable, (2.28) and (2.29) follow from dominated convergence.

$$\lim_{\mu \rightarrow -\infty} \rho(\mu) = 0 \quad (\text{SE2.7})$$

Solution E3

In the case of Fermions, each state can be occupied by at most one particle, so

$$\Xi = \prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \sum_{N_k=0}^1 e^{-\beta(\frac{k^2}{2m}-\mu)N_k} \equiv \prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left(1 + e^{-\beta(\frac{k^2}{2m}-\mu)}\right) \quad (\text{SE3.1})$$

and

$$\langle \mathcal{B}_q \rangle = \frac{1}{\Xi} e^{-\beta(\frac{q^2}{2m}-\mu)} \prod_{k \in \frac{2\pi}{L}\mathbb{Z}^3 \setminus \{q\}} \left(1 + e^{-\beta(\frac{k^2}{2m}-\mu)}\right) \quad (\text{SE3.2})$$

so

$$\langle \mathcal{B}_q \rangle = \frac{e^{-\beta(\frac{q^2}{2m}-\mu)}}{1 + e^{-\beta(\frac{q^2}{2m}-\mu)}} = \frac{1}{1 + e^{\beta(\frac{q^2}{2m}-\mu)}}. \quad (\text{SE3.3})$$

There cannot be Bose-Einstein condensation for Fermions, because each state can only be occupied by at most one particle, so it is not possible for a state to have an occupation number that is proportional to N .

Solution E4

For $r \leq R$,

$$\partial_r^2(r\psi) = mUr\psi \quad (\text{SE4.1})$$

so

$$r\psi = A \cosh(\sqrt{mUr}) + B \sinh(\sqrt{mUr}). \quad (\text{SE4.2})$$

For $r > R$,

$$\partial_r^2(r\psi) = 0 \quad (\text{SE4.3})$$

so, since $\psi \rightarrow 1$ as $r \rightarrow \infty$,

$$r\psi = r - a. \quad (\text{SE4.4})$$

Since $r\psi = 0$ at $r = 0$,

$$r\psi = B \sinh(\sqrt{mUr}) \quad (\text{SE4.5})$$

and since $r\psi$ is continuous at R ,

$$B = \frac{R - a}{\sinh(\sqrt{mUR})}. \quad (\text{SE4.6})$$

This implies (3.18).

Solution E5

By Theorem A1.15, e^{-tH_N} is positivity preserving. In addition, e^{-tH_N} is compact by Theorem A1.11, and the spectrum of e^{-tH_N} is $e^{-t \operatorname{spec}(H_N)}$, and the largest eigenvector of e^{-tH_N} with the largest eigenvalue is the ground-state of H_N . Finally, since $\operatorname{spec}(H_N) \geq 0$ (because $-\Delta \geq 0$ and $v \geq 0$), we can apply the Perron-Frobenius theorem, which implies that ψ_0 is unique and ≥ 0 .

Solution E6

The potential term $\int dx V(x)|\psi_0|^2$ is obviously the same for ψ_0 and $|\psi_0|$, so we only need to worry about the kinetic term. Let

$$P := \{x \in \mathbb{R}^{3N} : \psi_0(x) \neq 0\}. \quad (\text{SE6.1})$$

Now, ψ_0 is twice continuously differentiable, since it is an eigenfunction and v is continuous (see [LL01, Theorem 11.7(vi)]), so $|\psi_0|$ is twice continuously differentiable on P , and so

$$-\int dx |\psi_0| \Delta |\psi_0| \equiv -\int_P dx |\psi_0| \Delta |\psi_0| = \int_P dx (\nabla |\psi_0|)^2 + \int_{\partial P} dx |\psi_0(x)| (n(x) \cdot \nabla |\psi_0|) \quad (\text{SE6.2})$$

where $n(x)$ is the normal vector at x (∂P is differentiable because ψ_0 is as well), but since $\psi_0(x) = 0$ on ∂P ,

$$-\int dx |\psi_0| \Delta |\psi_0| = \int_P dx (\nabla |\psi_0|)^2 = \int_P dx \left(\nabla \psi_0 \frac{\psi_0}{|\psi_0|} \right)^2 = \int_P dx (\nabla \psi_0)^2 = -\int_P dx \psi_0 \Delta \psi_0. \quad (\text{SE6.3})$$

Thus, $\mathcal{E}(|\psi_0|) = \mathcal{E}(\psi_0)$. Since ψ_0 is the minimizer of $\mathcal{E}(\psi_0)$, so is $|\psi_0|$, but since the ground state is unique,

$$\psi_0 = |\psi_0| \quad (\text{SE6.4})$$

so $\psi_0 \geq 0$.

Solution E7

Let $\tilde{\psi}_0(\epsilon)$ denote the ground state of $\tilde{H}_N(\epsilon)$ with $\|\tilde{\psi}_0(\epsilon)\|_2 = 1$. We have

$$\tilde{E}_0(\epsilon) = \left\langle \tilde{\psi}_0(\epsilon) \left| \tilde{H}_N(\epsilon) \right| \tilde{\psi}_0(\epsilon) \right\rangle \quad (\text{SE7.1})$$

so

$$\partial_\epsilon \tilde{E}_0|_{\epsilon=0} = 2 \left\langle \partial_\epsilon \tilde{\psi}_0|_{\epsilon=0} \left| H_N \right| \psi_0 \right\rangle + \langle \psi_0 | \partial_\epsilon \tilde{H}_N|_{\epsilon=0} | \psi_0 \rangle \quad (\text{SE7.2})$$

that is

$$\partial_\epsilon \tilde{E}_0|_{\epsilon=0} = 2E_0 \left\langle \partial_\epsilon \tilde{\psi}_0|_{\epsilon=0}, \psi_0 \right\rangle + \langle \psi_0 | \sum_{i=1}^N P_i | \psi_0 \rangle. \quad (\text{SE7.3})$$

In addition,

$$2 \left\langle \partial_\epsilon \tilde{\psi}_0|_{\epsilon=0}, \psi_0 \right\rangle = \partial_\epsilon \left\langle \tilde{\psi}_0(\epsilon), \tilde{\psi}_0(\epsilon) \right\rangle |_{\epsilon=0} = \partial_\epsilon 1|_{\epsilon=0} = 0. \quad (\text{SE7.4})$$

Thus,

$$\frac{1}{N} \partial_\epsilon \tilde{E}_0|_{\epsilon=0} = \frac{1}{N} \sum_{i=1}^N \langle \psi_0 | P_i | \psi_0 \rangle. \quad (\text{SE7.5})$$