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Arbeitsgemeinschaft: Analysis of Many-body Quantum Systems

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Abstract. This Oberwolfach Arbeitsgemeinschaft focuses on the mathematical analysis of quantum many-body systems. Of particular interest is the ground state energy of dilute quantum gases, either fermions or bosons, and its low-density expansion in the thermodynamic limit.

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Introduction by the Organizers

The understanding of many-body systems in quantum mechanics is a central aspect of Mathematical Physics. Recent technological advances in trapping and cooling atoms allowed to explore many fascinating aspects of such systems, including phenomena like superfluidity and Bose–Einstein condensation. Partly motivated by this progress, there has been a substantial effort in the past two decades to develop new mathematical tools to solve some of the outstanding open problems in this field. The goal of this workshop was to give a comprehensive overview of some of the techniques that have been developed, as well as the kind of problems that have been successfully attacked.

The particles to be considered are either *bosons* or *fermions*, and their mathematical description differs significantly. Both finite, trapped systems and extended systems in the thermodynamic limit are being considered. The focus is at zero temperature (i.e., the ground state and low-lying excitations), even though some of the results can also be extended to the case of positive temperature.

The various lectures during the Arbeitsgemeinschaft can be divided into four groups. The first four lectures on the first day set the stage for the mathematical formulation of quantum many-body or many-particle physics. Many particle systems are described by tensor products of the Hilbert spaces of the one-particle spaces. The identical particles under consideration are either bosons or fermions, where the symmetric or anti-symmetric tensor products appear. The interactions considered are two-body, i.e., sums of terms that involve only two particles (i.e., operators acting on tensor products of two one-particle spaces).

The combinatorics for many-particle systems is complicated. The first lecture introduces the method of 2nd quantization, in particular, creation and annihilation operators, that greatly simplifies the combinatorics. The creation and annihilation operators satisfy either canonical commutation relations (Bosons) or canonical anti-commutation relations (Fermions). The many-body Hamiltonians describing many-particle systems with two-body interactions are quartic polynomials in creation and annihilation operators. The second lecture considers the treatment of operators that are quadratic polynomials in creation and annihilation operators. Many such operators can be diagonalized using what is referred to as unitary coherent translations and Bogoliubov unitary transformations. The ground states of quadratic Hamiltonians define the class of quasi-free or Gaussian states. These states may also be characterized as those satisfying that expectations of monomials in creation and annihilation operators may be calculated from expectations of quadratic monomials using Wick's Theorem. The third lecture discusses the simplest approximation of bosonic quartic operators in terms of quadratic operators in what is referred to as the mean-field limit. The approximation is relevant both for the ground state and the low-lying excited states. Even if the quartic operator is particle number preserving (all terms are products of equal numbers of creation and annihilation operators) the best quadratic approximation may not be. This may sound meaningless, but can be understood by mapping to a different space where particle number is not preserved. This is important in the proof of the approximation and is covered in the forth lecture.

The lectures on the second day focus on dilute Bose gases. The first two lectures discuss the ground state energy per unit volume $e(\rho)$ of a dilute Bose gas in the thermodynamic limit, where the number of particles and the volume tend to infinity, at fixed density $\rho > 0$. Denoting by $a > 0$ the scattering length of the two-body interaction, it is shown that $e(\rho) \simeq 4\pi a\rho^2$, up to corrections that are of smaller order in the limit $\rho a^3 \to 0$. The first lecture discusses the precise definition of the scattering length and proves an upper bound for $e(\rho)$, estimating the energy of an appropriate trial state. In the second lecture, a matching lower bound is shown, following the work of Lieb and Yngvason. An important tool to reach this goal is a lemma, going back to Dyson, that allows to replace the interaction among the particles by a new potential, with smaller size and longer range, which can then be treated as a perturbation of the kinetic energy. The following two lectures then discuss the Gross–Pitaevskii limit, where N bosons are confined in the three dimensional unit torus and interact through a repulsive potential with effective range of the order $1/N$. After rescaling, the Gross–Pitaevskii regime describes a very dilute Bose gas, with density converging to 0, in the limit of large N. In this regime, low-energy states are known to exhibit complete Bose–Einstein condensation, i.e., most particles occupy the same one-particle state (in the translation invariant setting, the zero momentum state).

The two lectures on Wednesday morning focus on the Lee–Huang–Yang formula, which is the next correction to the leading term $e(\rho) \simeq 4\pi a\rho^2$ mentioned above. The lectures present the main ideas and steps for proving the validity of the Lee–Huang–Yang formula both as an upper and a lower bound.

The two lectures on Thursday morning present the corresponding analysis for Fermi gases, i.e., an asymptotic expansion of the ground state energy at low density. An important difference compared to the bosonic case concerns the fact that the leading term (i.e., the one in the absence of any interaction) is non-vanishing for fermions, hence the leading contribution from the interactions (the analogue of the $4\pi a\rho^2$ for bosons) is here the first correction term. The next correction is known as the Huang–Yang term, and the lectures will introduce the main ideas in the recent proof of its validity.

The final three lectures focus on fermions at high density. The first lecture Thursday afternoon explains the semiclassical approximation for fermionic systems. As a particularly relevant example, it discusses the validity of the Thomas–Fermi density functional for the ground state energy of heavy atoms, as originally proved by Lieb and Simon. More modern approaches utilize the Lieb–Thirring and Lieb–Oxford inequalities, which are being discussed. The second lecture investigates the validity of the Hartree–Fock approximation. In particular, it discusses the method of Graf and Solovej to bound the correlation energy of a charged Fermi gas ("jellium") at high density. The last lecture on Friday morning focuses on the random-phase approximation, which for fermions at high density leads to a prediction of the leading term in the correlation energy, i.e., the correction to the Hartree–Fock approximation. Recently this problem was solved in a mean-field approximation (more precisely, it is really a combined semi-classical mean-field limit) for translation-invariant systems on the torus. The lecture focuses on the basic heuristics of the approximation, as well as a sketch of the proof of the upper bound to the correlation energy.

The workshop was closed by a summary, given by the organizers, of the main topics covered, giving also an outlook on possible future directions as well as open problems in the field.

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Arbeitsgemeinschaft: Analysis of Many-body Quantum Systems

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Abstracts

Fock space, creation and annihilation operators, Hamiltonians, and density matrices

Jan Philip Solovej

This first lecture of the week was, as all the other lectures, supposed to have been given by one of the participants. Unfortunately, the participant could not make it and the lecture was therefore given by an organizer.

The lecture introduced the basic formalism of many-body quantum theory. The Hilbert space for several particles is given by the tensor product of the one-body spaces. In the case of identical particles, the physically most relevant cases are to either restrict to the symmetric subspace (bosons) or to the anti-symmetric subspace (fermions). To get a full description of the many-body systems we also need the Hamiltonian. The simplest case is the situation where the particles are non-interacting. In this case the non-interacting Hamiltonian is simply the sum of the one-body Hamiltonians acting on the individual particles. It is more interesting to consider interacting Hamiltonians. In this talk as in most of the other lectures we focus on two-body interactions acting on two particles at a time, i.e., acting in the two-particle Hilbert space. An interacting Hamiltonian then consists of the non-interacting part plus an interacting term formed by summing over all pairs of the two-body interaction. The talk described the ground state energy (bottom of the spectrum) of the non-interacting Hamiltonians.

For bosons, it is easy as it is simply the number of particles, say N, times the ground state energy of the one-body Hamiltonian. For fermions, it is the sum of the first N lowest eigenvalue of the one-body Hamiltonian reflecting the Pauli exclusion principle. The talk also introduced the positive temperature free energy in terms of the entropy of a quantum state.

To calculate the free energy of the non-interacting system it was convenient to introduce the bosonic and fermionic Fock spaces and second quantization described by creation and annihilation operators. Using those it was not difficult to find the free energy for non-interacting fermions or bosons, although this required considering the grand canonical picture in which the particle number is not kept fixed, but a chemical potential is introduced. The talk went on to show how to write the interacting Hamiltonian in terms of the creation and annihilation operators and how to naturally introduce the one-particle reduced density matrix in terms of creation and annihilation operators. Elementary properties of the one-particle reduced density matrix were given. They included the positivity and trace condition for both fermions and bosons. We also proved that the one-particle reduced density matrix for fermions is bounded by one (the Pauli principle). Many of these concepts were developed further in later lectures.

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Quadratic Hamiltonians, Quasi-Free States, and Bogoliubov Transforms

Daniele Ferretti

In the framework of second quantization, Bogoliubov's theory pivots on finding appropriate ways to neglect the cubic and quartic terms (with respect to the creation and annihilation operators) of a given self-adjoint operator. This shifts the focus to the quadratic contributions and how to deal with them. Specifically, one needs a robust construction allowing one to obtain a diagonal representation of such quadratic terms so that the excitation spectrum can be understood in terms of quasi-particles contributions plus error terms.

In this talk, we discussed the necessary notions to understand this machinery. To this end, given a complex, separable Hilbert space $\mathfrak{h}$, we introduced the generalized creation and annihilation operators

$$A_\pm(f \oplus g) = a_\pm(f) + a_\pm^*(Jg)$$

on the ($+$: bosonic, $-$: fermionic) Fock space $\mathfrak{F}_\pm(\mathfrak{h})$ built over $\mathfrak{h}$, where $g, f \in \mathfrak{h}$, and J is a conjugation map (an anti-unitary involution) from $\mathfrak{h}$ to $\mathfrak{h}$. These quantities serve to define the generalized one-particle density matrix Γ_ρ of a given mixed state ρ, for which the expected number of particles is finite. Such Γ_ρ is the self-adjoint, non-negative, trace-class operator on $\mathfrak{h} \oplus \mathfrak{h}$ satisfying

$$\langle F, \Gamma_\rho\, G\rangle_{\mathfrak{h}\oplus\mathfrak{h}} = \mathrm{Tr}\,(A_\pm^*(G)A_\pm(F)\,\rho), \qquad F, G \in \mathfrak{h} \oplus \mathfrak{h}.$$

In this framework, a Bogoliubov map $\mathcal{V}$ is an isomorphism on $\mathfrak{h} \oplus \mathfrak{h}$ commuting with

$$\mathcal{J} := \begin{bmatrix} 0 & J \\ J & 0 \end{bmatrix}$$

and preserving the canonical (anti-)commutation relations

$$A_\pm(F)A^*(G) \mp A_\pm^*(G)A(F) = \langle F, S_\pm G\rangle_{\mathfrak{h}\oplus\mathfrak{h}}, \qquad S_\pm := \begin{bmatrix} \mathbb{1}_\mathfrak{h} & 0 \\ 0 & \mp\mathbb{1}_\mathfrak{h} \end{bmatrix}.$$

We discussed the properties and implementability of a Bogoliubov map on a given Fock space, namely, the existence of a unitary operator $\mathbb{U}_\mathcal{V}$ – a Bogoliubov transform – on $\mathfrak{F}_\pm(\mathfrak{h})$ such that $\mathbb{U}_\mathcal{V}\,\Omega$ has a finite expected number of particles (with Ω the vacuum), and

$$\mathbb{U}_\mathcal{V} A_\pm(F)\mathbb{U}_\mathcal{V}^* = A_\pm(\mathcal{V}F), \qquad \forall F \in \mathfrak{h} \oplus \mathfrak{h}.$$

We also emphasized the role of the Shale-Stinespring condition.

Then, we introduced the notion of a quasi-free state as any self-adjoint, non-negative, unit trace operator on $\mathfrak{F}_\pm(\mathfrak{h})$ satisfying the Wick rule in terms of the generalized creation/annihilation operators. We stressed that the set of quasi-free states is invariant under Bogoliubov transforms – that is, if G is quasi-free then $\mathbb{U}_{\mathcal{V}}\, G\, \mathbb{U}_{\mathcal{V}}^*$ is quasi-free as well. We also characterized pure quasi-free states Ψ as applications of Bogoliubov transforms on the vacuum $\mathbb{U}_{\mathcal{V}}\, \Omega$. In this case, the associated generalized one-particle density matrix must satisfy

$$\Gamma_{|\Psi\rangle\langle\Psi|}\, S_\pm\, \Gamma_{|\Psi\rangle\langle\Psi|} = \mp \Gamma_{|\Psi\rangle\langle\Psi|}.$$

We recalled the definition of the second quantization of a one-particle operator and the representation of its associated quadratic form in terms of creation and annihilation operators.

We then generalized this construction by introducing a quadratic Hamiltonian $\mathcal{H}^\pm_{\mathcal{A}}$ associated with a self-adjoint trace-class operator $\mathcal{A}$ on $\mathfrak{h} \oplus \mathfrak{h}$. This generalization involves all possible combinations of two creation and/or annihilation operators, instead of just $a^*_\pm a_\pm$. We required $\mathcal{A}$ to be positive definite in the bosonic case. The quadratic Hamiltonian $\mathcal{H}^\pm_{\mathcal{A}}$ has been defined as

$$\mathcal{H}^\pm_{\mathcal{A}} = \sum_{i,j\in \mathbb{N}} \langle F_i, \mathcal{A} F_j\rangle_{\mathfrak{h}\oplus\mathfrak{h}} A^*_\pm(F_i) A_\pm(F_j), \qquad \{F_i\}_{i\in\mathbb{N}} \text{ basis of } \mathfrak{h}\oplus\mathfrak{h},$$

with the truncated Fock space $\mathfrak{F}^0_\pm(\mathfrak{h})$ as a core domain. We proved that this definition is independent of the chosen basis and that $\mathcal{H}^\pm_{\mathcal{A}}$ admits a unique self-adjoint extension. Moreover, for any φ in the domain of the Hamiltonian,

$$\langle \varphi, \mathcal{H}^\pm_{\mathcal{A}}\, \varphi\rangle_{\mathfrak{F}_\pm(\mathfrak{h})} = \mathrm{Tr}\,(\mathcal{A}\, \Gamma_{|\varphi\rangle\langle\varphi|}).$$

Furthermore, for any implementable Bogoliubov map $\mathcal{V}$

$$\mathbb{U}_{\mathcal{V}}\, \mathcal{H}^\pm_{\mathcal{A}}\, \mathbb{U}_{\mathcal{V}}^* = \mathcal{H}^\pm_{\mathcal{V}\mathcal{A}\mathcal{V}^*}.$$

Without loss of generality, one can assume $\mathcal{A}$ satisfies

(i) $$\mathcal{J}\mathcal{A}\,\mathcal{J} = \pm\mathcal{A},$$

since there exists $\mathcal{A}'$ self-adjoint, trace-class (positive definite for bosons), and satisfying (i), for which one has

$$\mathcal{H}^\pm_{\mathcal{A}'} = \mathcal{H}^\pm_{\mathcal{A}} \pm \frac{1}{2}\,\mathrm{Tr}\,(\mathcal{A}\, S_\pm)\, \mathbb{1}_{\mathfrak{F}_\pm(\mathfrak{h})}.$$

This property is crucial, as we exhibited a theorem stating that for $\mathcal{A}$ bounded, self-adjoint, satisfying (i) (positive definitive for bosons), and such that $S_\pm\mathcal{A}$ has a basis of eigenvectors, there exists an implementable Bogoliubov map $\mathcal{V}$ such that $\mathcal{V}^*\mathcal{A}\mathcal{V}$ is diagonal with eigenvectors $\{u_n \oplus 0\}_{n\in\mathbb{N}} \cup \{0 \oplus Ju_n\}_{n\in\mathbb{N}}$ forming a basis of $\mathfrak{h}\oplus\mathfrak{h}$. Plugging this specific basis into the expression for $\mathbb{U}_{\mathcal{V}^*}\mathcal{H}^\pm_{\mathcal{A}}\,\mathbb{U}^*_{\mathcal{V}^*}$, we find that it can be written as the second quantization of a self-adjoint, compact one-particle operator on $\mathfrak{h}$. We also mentioned that a similar result can be obtained by relaxing the assumption that $\mathcal{A}$ is trace-class; however, the proof in this case requires a much richer structure, and the definition of the quadratic Hamiltonian must omit the $a_\pm a^*_\pm$ terms.

In conclusion, we argued that the ground state of a quadratic Hamiltonian (if it exists) is a pure quasi-free state.

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Mean-field limit for bosons & Bogoliubov approximation

Yoann Le Hénaff

In this lecture we will present the Bogoliubov approximation, which is at the heart of the Bogoliubov theory. The aim is to give the intuitive ideas behind this theory in a clear but non-rigorous manner, before Jinyeop Lee proves rigorously the technical details in the next talk.

To make the heuristics more understandable, we consider a simple physical setting. More precisely, we use a box $\Omega = [0,1]^d$, $d \geq 1$, with periodic boundary conditions, containing N particles subject to the Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \text{ acting on } L^2_s(\Omega^N).$$

We consider here symmetric functions, i.e. a bosonic system, though the ideas are exactly the same for fermions. We focus on the mean-field regime, but the ideas we present work for other regimes, including the thermodynamic limit and Gross–Pitaevskii.

The potential is assumed to be:

- real-valued, i.e. $V : \mathbb{R}^d \to \mathbb{R}$,
- periodic, with period 1: $V(x+n) = V(x)$ for $\forall n \in \mathbb{Z}^d$, $x \in \Omega$,
- bounded: $\|V\|_\infty < \infty$,
- semi-positive definite: $\hat{V}(k) \geq 0$, $\forall k \in 2\pi\mathbb{Z}^d$, where

$$\hat{V}(k) := \int_\Omega V(x) e^{-ik\cdot x} dx.$$

The Bogoliubov theory can be used to estimate the ground state energy of a particle system in the case of interactions, defined by

$$E_N := \inf_{\psi \in L^2_s(\Omega^N):\ \|\psi\|_{L^2} = 1} \langle \psi | H_N \psi \rangle .$$

The first part of the lecture is about finding the ground state energy of the system in the noninteracting case $V \equiv 0$. It can be shown that $E_N = 0$, and a minimizer is $\psi_N^0 = \varphi_0 \otimes \cdots \otimes \varphi_0$ with $\varphi_0 \equiv 1$ on Ω.

The second part of the lecture consists in obtaining an estimate for the ground state energy in the interacting case $V \not\equiv 0$. A first estimate of E_N can be obtained in a straightforward manner by obtaining lower and upper bounds, yielding

$$\left|\frac{N}{2}\hat{V}(0) - E_N\right| \leq C.$$

The upper bound is obtained by using ψ_N^0 as a trial state, and the lower bound comes from a lower bound on V that one can obtain using our assumptions. The lower bound on V can also be used to show that, for wave functions with an energy that remain a constant away from E_N for all N, there is condensation in the state φ_0 as $N \to \infty$. The above estimate of E_N is of order $\mathcal{O}(N)$. To obtain a more precise value, we use the formalism of second quantization using the creation and annihilation operators a_p^*, a_p associated to the Fourier mode of frequency p. We recall that $a_p^* a_p$ is the operator that counts the number of particles in the Fourier mode of frequency p.

The essential idea from Bogoliubov is that, since one expects condensation in the state φ_0 (which is the Fourier mode of frequency 0), one should have $a_0^* a_0 \psi_N \approx N\psi_N$. The operators a_0^*, a_0 don't commute, however $[a_0, a_0^*] = 1 \ll N$. Hence, compared to N, the non-commutability is negligible. Bogoliubov suggests treating these operators as scalars, with $a_0 = a_0^* = \sqrt{N_0}$ and N_0 the number of particles in the state φ_0. After writing the second quantization of the Hamiltonian H_N and replacing every occurrence of the operators a_0, a_0^* with $\sqrt{N_0}$, one obtains an expression with products of two, three, and four creation and annihilation operators. It can be shown that the terms involving products of three and four such operators are of order $N^{-1/2}$, thus become negligible as $N \to \infty$.

In order to treat the products of two creation and annihilation operators, we introduce modified creation and annihilation operators b_p^*, b_p, such that the quadratic part of the second quantized version of H_N becomes diagonal – in the sense that it only involves products of the form $b_p^* b_p$. By writing the Hamiltonian using these new operators, a constant of order $\mathcal{O}(1)$ appears. Finally, the improved estimate of E_N is the addition of the $\mathcal{O}(N)$ and $\mathcal{O}(1)$ estimates of E_N, and other terms in the Hamiltonian vanish as $N \to \infty$.

The theory and computations are the same for bosonic and fermionic systems, up to the definition of the modified operators: these operators b_p^*, b_p have either to satisfy the CCR (in the case of bosons) or CAR (in the case of fermions).

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Rigorous Derivation of Bogoliubov Theory for Bose Gases in the Mean-Field Regime

Jinyeop Lee

Bogoliubov theory describes low energy excitations of weakly interacting Bose gases by approximating the many-body Hamiltonian with an effective quadratic operator on Fock space. While the physical picture of this approximation is well understood, establishing it rigorously in the mean-field regime remains subtle. In this talk, I follow the approach presented in Schlein's lecture note and discuss how to make the Bogoliubov approximation rigorous, with quantitative control of the error terms.

We consider N bosons on the unit torus $\Lambda := [-\frac{1}{2}, \frac{1}{2}]^3$, interacting via a positive definite potential $V \in L^1(\mathbb{R}^3)$ with compact support, whose Fourier coefficients are denoted by $\widehat{V}(p)$, $p \in 2\pi\mathbb{Z}^3$. The Hamiltonian is

$$H_N = \sum_{j=1}^{N}(-\Delta_{x_j}) + \frac{1}{N}\sum_{1\le i<j\le N} V(x_i - x_j),$$

acting on the symmetric subspace $L^2_s(\Lambda^N)$, with ground state energy E_N. In the mean-field limit, particles are interacting weakly with all others, so that the leading contribution to E_N is

$$E_N \simeq \frac{N-1}{2}\widehat{V}(0).$$

The next order correction of order one, predicted by Bogoliubov theory, describes collective excitations above the condensate.

Following Seiringer [1], Lewin–Nam–Serfaty–Solovej [2], and Schlein [3], we introduce a unitary map U_N that factors out the condensate and acts on the truncated excitation Fock space $\mathcal{F}_{\le N}^{\perp\varphi_0}$. The many-body Hamiltonian transforms into an *excitation Hamiltonian*

$$\mathcal{L}_N = \mathcal{L}_N^{(0)} + \mathcal{L}_N^{(2)} + \mathcal{L}_N^{(3)} + \mathcal{L}_N^{(4)},$$

where $\mathcal{L}_N^{(k)}$ collects terms of order k in the modified creation and annihilation operators b_p^*, b_p. A key ingredient is a quantitative condensation estimate:

$$\langle \psi_N, (\mathcal{K}_+ + 1)(\mathcal{N}_+ + 1)\psi_N\rangle \le C,$$

where $\mathcal{N}_+$ counts excitations and $\mathcal{K}_+$ is the kinetic energy of nonzero modes. This bound implies that the cubic and quartic contributions $\mathcal{L}_N^{(3)}$, $\mathcal{L}_N^{(4)}$ are negligible on low-energy states.

Neglecting higher-order terms, as justified by the above bound, we obtain the *effective quadratic operator*

$$\mathcal{L}_N \simeq \frac{N-1}{2}\widehat{V}(0) + \sum_{p\neq 0}(|p|^2 + \widehat{V}(p))b_p^* b_p + \frac{1}{2}\sum_{p\neq 0}\widehat{V}(p)(b_p^* b_{-p}^* + b_p b_{-p}),$$

up to an error of order $N^{-1/2}$. It can be diagonalized by a generalized Bogoliubov transformation $T = \exp\big[\frac{1}{2}\sum_{p\neq 0}\eta_p(b_p^* b_{-p}^* - b_p b_{-p})\big]$, where $\tanh(2\eta_p) = -\widehat{V}(p)/(|p|^2+\widehat{V}(p))$. Conjugation yields

$$T^*\mathcal{L}_N T = \frac{N-1}{2}\widehat{V}(0) + \frac{1}{2}\sum_{p\neq 0}\Big[(|p|^2+\widehat{V}(p)) - \sqrt{|p|^4+2|p|^2\widehat{V}(p)}\Big] + \sum_{p\neq 0}\sqrt{|p|^4+2|p|^2\widehat{V}(p)}\, a_p^* a_p + \mathcal{E}_N,$$

with $\pm\mathcal{E}_N \leq CN^{-1/2}$. Hence,

$$E_N = \frac{N-1}{2}\widehat{V}(0) + \frac{1}{2}\sum_{p\neq 0}\Big[(|p|^2+\widehat{V}(p)) - \sqrt{|p|^4+2|p|^2\widehat{V}(p)}\Big] + \mathcal{O}(N^{-1/2}),$$

and the low-lying excitation spectrum is given by

$$\sum_{p\neq 0} n_p\sqrt{|p|^4+2|p|^2\widehat{V}(p)} + \mathcal{O}(N^{-1/2}), \qquad n_p\in\mathbb{N}.$$

Thus, the rigorous spectrum coincides with Bogoliubov's prediction up to vanishing errors as $N\to\infty$.

This analysis provides a mathematically rigorous derivation of Bogoliubov theory for mean-field Bose gases, combining the Fock space formalism, excitation estimates, and an exact diagonalization of the quadratic Hamiltonian. The argument presented here closely follows the derivation outlined in B. Schlein's lecture note, with inspiration from Seiringer's and Lewin–Nam–Serfaty–Solovej's earlier works.

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Upper bound on the ground state energy of the dilute Bose gas

Severin Schraven

The purpose of this talk is to explain the upper bound on the ground state energy of a dilute Bose gas in the thermodynamic limit. We consider a bosonic gas of N particles in the box $\Lambda_L = [-L/2, L/2]^3$ (with periodic boundary conditions) interacting through a hard-sphere potential and are interested in its ground state energy. This means, we wish to study the quantity

$$E_{L,N} = \inf\frac{\langle\psi_N, \sum_{j=1}^N -\Delta_{x_j}\psi_N\rangle}{\|\psi_N\|^2}, \tag{1}$$

where the infimum is taken over all $\psi_N \in L^2(\Lambda_L^N)$ which are symmetric, i.e. $\psi_N(x_1,\dots,x_N) = \psi_N(x_{\sigma(1)},\dots,x_{\sigma(N)})$ for all permutations $\sigma \in S_N$, and which satisfy the hard-core condition;

$$\psi_N(x_1,\dots,x_N) = 0 \qquad \text{if} \qquad \min_{i\neq j} |x_i - x_j| < \mathfrak{a}. \tag{2}$$

We fix a density $\rho > 0$ and consider the thermodynamic limit $N, L \to \infty$ with $N/L^3 = \rho$. The energy per particle is then defined by

$$e(\rho) = \lim_{N,L\to\infty, N/L^3=\rho} \frac{E_{L,N}}{N}. \tag{3}$$

It was conjectured by Lee-Huang-Yang [12] that for the dilute regime we have

$$e(\rho) = 4\pi\mathfrak{a}\rho\left(1 + \frac{128}{15\sqrt{\pi}}(\rho\mathfrak{a}^3)^{1/2} + o((\rho\mathfrak{a}^3)^{1/3})\right), \qquad \rho\mathfrak{a}^3 \to 0. \tag{4}$$

The first rigorous result was obtained by Dyson [8], who obtained the correct upper bound to leading order. More than forty years later, Lieb-Yngvason [13] proved the matching lower bound of the leading order. Combined they showed

$$e(\rho) = 4\pi\mathfrak{a}\rho(1 + o(1)), \qquad \rho\mathfrak{a}^3 \to 0. \tag{5}$$

While much is known in the case of less singular potentials or lower bounds, see [14, 9, 1, 10, 6] and references therein, there is currently no upper bound capturing the second term in (4) for hard-sphere potentials. Currently, the best known result, [2], is an upper bound for hard-spheres where the second term is of the correct order, i.e. $(\rho\mathfrak{a}^3)^{1/2}$, but with the wrong constant. It remains an important open problem to establish such an upper bound with the correct constant.

Let us sketch the idea of the proof, following the presentation in [3]. As we are trying to find an upper bound on the ground state energy (1), we have to come up with a suitable trial state. In the free case, i.e. $\mathfrak{a} = 0$ the minimizer of (1) is explicitely known, it is a constant function. In the general case our trial state will need to encode correlations too. We choose it to be of the form

$$\Psi_N(x_1,\dots,x_N) = \prod_{1\le i<j\le N} f_\ell(x_i - x_j). \tag{6}$$

This is called a Bijl-Dingle-Jastrow factor due to [5, 7, 11]. The function f_ℓ is meant to capture correlation between two particles on a length scale $\mathfrak{a} \ll \ell \ll L$, which we choose later. Furthermore, on larger scales, the function f_ℓ should be equal to the minimizer of the free problem.

We define f_ℓ to be the ground state of the Neumann problem on the ball of radius ℓ which also satisfies the hard-sphere condition (2), i.e. we want

$$\begin{cases} -\Delta f_\ell &= \lambda_\ell f_\ell, \\ \partial_r f_\ell(x) &= 0, \quad |x| = \ell, \\ f_\ell(x) &= 0, \quad |x| = \mathfrak{a}. \end{cases} \tag{7}$$

The solution will be radially symmetric, and we normalize the eigenfunction such that $f_\ell(x) = 1$ for $|x| = \ell$. Furthermore, we will extend f_ℓ by 1 to all of Λ_L. In the following we will denote by χ_ℓ the indicator function of the ball of radius ℓ centered at zero. One has the following key estimates

Lemma 1. [3, Lemma 2.1] *For $\mathfrak{a} \ll \ell$ we have*

$$\lambda_\ell = \frac{3\mathfrak{a}}{\ell^3}\left(1 + \mathcal{O}(\mathfrak{a}/\ell)\right), \tag{8}$$

and

$$|\nabla f_\ell(x)| = C\mathfrak{a}\frac{\chi_\ell(x)}{|x|^2}, \qquad 0 \le 1 - f_\ell(x)^2 \le C\mathfrak{a}\frac{\chi_\ell(x)}{|x|}. \tag{9}$$

We now estimate the energy of the normalized trial state (6). For fixed $j \in \{1, \ldots, N\}$ we have

$$\begin{aligned}\frac{-\Delta_{x_j}\Psi_N(x_1,\ldots,x_N)}{\prod\limits_{1\le j<k\le N} f_\ell(x_j - x_k)} &= \sum_{i=1, i\neq j}^{N} \frac{-\Delta f_\ell(x_j - x_i)}{f_\ell(x_j - x_i)} - \sum_{\substack{i,m=1\\ i,m\neq j, m\neq i}}^{N} \frac{\nabla f_\ell(x_j - x_i)}{f_\ell(x_j - x_i)} \cdot \frac{\nabla f_\ell(x_j - x_m)}{f_\ell(x_j - x_m)} \\ &= \sum_{i=1, i\neq j}^{N} \lambda_\ell \chi_\ell(x_j - x_i) - \sum_{\substack{i,m=1\\ i,m\neq j, m\neq i}}^{N} \frac{\nabla f_\ell(x_j - x_i)}{f_\ell(x_j - x_i)} \cdot \frac{\nabla f_\ell(x_j - x_m)}{f_\ell(x_j - x_m)},\end{aligned}$$

where we have used (7) for the last equality. Thus, for $x = (x_1, \ldots, x_N)$ we get

$$\begin{aligned}\langle \Psi_N, \sum_{j=1}^{N} -\Delta_{x_j}\Psi_N\rangle = 2\lambda_\ell &\sum_{1\le i<j\le N} \int_{\Lambda_L^N} \chi_\ell(x_i - x_j) \prod_{1\le s<t\le N} f_\ell(x_s - x_t)^2 dx \\ &- \sum_{\substack{i,j,m=1\\ \text{all different}}}^{N} \int_{\Lambda_L^N} \frac{\nabla f_\ell(x_j - x_i)}{f_\ell(x_j - x_i)} \cdot \frac{\nabla f_\ell(x_j - x_m)}{f_\ell(x_j - x_m)} \prod_{1\le s<t\le N} f_\ell(x_s - x_t)^2 dx.\end{aligned}$$

By permutation symmetry, we get

$$\begin{aligned}\frac{\langle \Psi_N, \sum_{j=1}^N -\Delta_{x_j}\Psi_N\rangle}{\|\Psi_N\|^2} =& N(N-1)\lambda_\ell \frac{\int_{\Lambda_L^N} \chi_\ell(x_1 - x_2) \prod\limits_{1\le i<j\le N} f_\ell(x_i - x_j)^2 dx}{\int_{\Lambda_L^N} \prod\limits_{1\le i<j\le N} f_\ell(x_i - x_j)^2 dx} \\ &- \int_{\Lambda_L^N} \frac{\nabla f_\ell(x_1 - x_2)}{f_\ell(x_1 - x_2)} \cdot \frac{\nabla f_\ell(x_1 - x_3)}{f_\ell(x_1 - x_3)} \prod_{1\le i<j\le N} f_\ell(x_i - x_j)^2 dx \\ &\cdot \left(\int_{\Lambda_L^N} \prod_{1\le i<j\le N} f_\ell(x_i - x_j)^2 dx\right)^{-1} N(N-1)(N-2) \\ =:& A + B.\end{aligned}$$

The key problem is that it is difficult to compute $\|\Psi_N\|^2$. To circumvent this issue one estimates those fractions in such a fashion that cancellation of factors in the numerator and denominator occur.

Using $0 \leq f_\ell(x) \leq 1$, we have

$$\int_{\Lambda_L^N} \chi_\ell(x_1 - x_2) \prod_{1\leq i<j\leq N} f_\ell(x_i - x_j)^2 dx \leq \int_{\Lambda_L^N} \chi_\ell(x_1 - x_2) \prod_{2\leq i<j\leq N} f_\ell(x_i - x_j)^2 dx$$
$$= \frac{4}{3}\pi\ell^3 \int_{\Lambda_L^{N-1}} \prod_{2\leq i<j\leq N} f_\ell(x_i - x_j)^2 dx_2 \ldots dx_N.$$

We set $u_\ell(x) = 1 - f_\ell(x)^2$. Then, using again $0 \leq f_\ell(x) \leq 1$, we get

$$1 - \sum_{j=2}^{N} u_\ell(x_1 - x_j) \leq \prod_{j=2}^{N} f_\ell(x_1 - x_j) \leq 1. \tag{10}$$

Hence, we obtain

$$\int_{\Lambda_L^N} \prod_{1\leq i<j\leq N} f_\ell(x_i - x_j)^2 dx \geq \int_{\Lambda_L^N} \left(1 - \sum_{j=2}^{N} u_\ell(x_1 - x_j)\right) \prod_{2\leq i<j\leq N} f_\ell(x_i - x_j)^2 dx$$
$$\geq \left(L - C\mathfrak{a}N \int_{\Lambda_L} \frac{\chi_\ell(x_1)}{|x_1|} dx_1\right) \int_{\Lambda_L^{N-1}} \prod_{2\leq i<j\leq N} f_\ell(x_i - x_j)^2 dx_2 \ldots dx_N.$$

This readily implies, for $\mathfrak{a}/\ell, \mathfrak{a}\rho\ell^2 \ll 1$

$$A \leq N^2 \frac{3\mathfrak{a}}{\ell^3} \left(1 + \mathcal{O}(\mathfrak{a}/\ell)\right) \frac{\frac{4}{3}\pi\ell^3}{L^3 - CaN\ell^2} = 4\pi\mathfrak{a}N\rho \frac{1 + \mathcal{O}(\mathfrak{a}/\ell)}{1 - C\mathfrak{a}\rho\ell^2}.$$

Similarly, one can show

$$|B| \leq C\mathfrak{a}N\rho \frac{\rho\mathfrak{a}\ell^2}{1 - C\rho\mathfrak{a}\ell^2}.$$

Note that in the limit we are interested, B is of subleading order compared to our estimate on A.

We now choose $\ell = \rho^{-1/3}$ (i.e. the mean inter-particle distance), then

$$\mathfrak{a}/\ell = (\rho\mathfrak{a}^3)^{1/3} = \rho\mathfrak{a}\ell^2.$$

In total, we get

$$\frac{E_{L,N}}{N} \leq 4\pi\mathfrak{a}\rho \left(1 + \mathcal{O}(\rho\mathfrak{a}^3)^{1/3}\right), \qquad \text{for } \rho\mathfrak{a}^3 \to 0. \tag{11}$$

This is precisely, the desired bound.

Note that (11) does not capture the second order term in the Lee-Huang-Yang formula (4). In [2] they give a modification of the proof which yields the correct scaling of the second order term. They use the same trial state, but pick a larger ℓ to capture more precise information on the correlations. More precisely, they use $\ell = c(\rho a)^{-1/2}$, for a sufficiently small $c > 0$. In this setting a more complicated combinatorial argument is needed to make use of cancellations.

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The leading order lower bound for the ground state energy of a 3D dilute Bose gas

Gabriele Ciccarello

The talk focused on the main ideas behind the proof by Lieb and Yngvason [2] of a leading order lower bound for the ground state energy of a three-dimensional dilute Bose gas in the thermodynamic limit. The exposition of the proof idea presented has been heavily inspired by [3], since it follows a more historical approach to the problem.

To be more precise, the following Hamiltonian was considered:

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

acting on $L^2(\Lambda)^{\otimes_s N}$, where Λ is a Neumann box with sidelength L and the potential is assumed to be radial, positive, and compactly supported. For such an operator, it is possible to prove the following theorem:

Theorem 1 (Lower Bound for the Ground State Energy of a 3D Dilute Bose gas)**.** *For a positive potential with compact support v, one has that the ground state energy of H_N with Neumann boundary conditions on the box satisfies:*

$$\frac{E_{GS}(N,L)}{N} \geq 4\pi\rho\mathfrak{a}(1 - C(\rho\mathfrak{a}^3)^{1/17}),$$

where $\mathfrak{a}$ is the scattering length associated with the potential v.

To illustrate what is required to prove such an estimate, the discussion began with *Dyson's lemma* and its corollary [1], which provide a way of softening the problem by lower bounding the full Hamiltonian with a nearest-neighbor type of potential: $H_N \geq \mathfrak{a}W$. It was shown, however, that this result alone is not sufficient: by sketching the proof of the original Dyson's lower bound for the hardcore potential, it was demonstrated that the correct order is obtained, but with the wrong constant.

The second step toward a correct proof involved lower bounding only *part* of the Hamiltonian to avoid sacrificing all of the kinetic energy. Specifically, the Hamiltonian was split as follows:

$$H_N = \varepsilon H_N + (1-\varepsilon)H_N \geq \varepsilon T_N + (1-\varepsilon)W =: \tilde{H}_N\,,$$

where T_N denotes the kinetic energy.

The form of $\tilde{H}_N$ suggested that perturbation theory techniques, such as *Temple's inequality*, could be applied. Unfortunately, this strategy was shown to be infeasible due to the large size of the box, which destroys the spectral gap required for Temple's inequality.

The final part of the talk addressed localization, justified by the spectral gap requirement. By dividing the thermodynamic box into smaller boxes of sidelength ℓ, a sharp lower bound for the ground state energy was derived. Particular attention was given to discussing the relevant length scales through the choice of the parameter ℓ.

The talk concluded with a heuristic derivation of the $4\pi\rho\mathfrak{a}$ energy density as the product of the energy of two particles in the large box and the total number of pairs.

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Condensation with Optimal Rate and Excitation Spectrum for Bose Gases in the Gross-Pitaevskii Limit

Jonas Köppl and Barbara Roos

We consider the Gross–Pitaevskii regime, where N Bosons are confined in the three-dimensional unit torus $\Lambda = [-1/2, 1/2]^3$ and interact through a repulsive pair potential V with scattering length $\mathfrak{a}$ of the order $1/N$. Denoting by ρ the density we have in particular $\rho\mathfrak{a}^3 = N^{-2}$, so the Gross–Pitaevskii limit describes very dilute Bose gases. The appropriately rescaled Hamiltonian is given by

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^2 V(N(x_i - x_j)) \tag{1}$$

and acts on the Hilbert space $L^2_s(\Lambda^N)$, defined as the subspace of $L^2(\Lambda^N)$ consisting of functions that are symmetric with respect to permutations. We assume that the potential $V \in L^2(\mathbb{R}^3)$ is non-negative, radial, and compactly supported. The scattering length of V can then be defined through the formula

$$4\pi\mathfrak{a} = \frac{1}{2}\int_{\mathbb{R}^3} V(x)dx - \left\langle \frac{1}{2}V, \frac{1}{-\Delta + \frac{1}{2}V}\frac{1}{2}V \right\rangle. \tag{2}$$

As first shown in [16] the ground state energy E_N of the Hamiltonian (1) satisfies

$$E_N = 4\pi\mathfrak{a}N + o(N) \quad \text{as } N \to \infty. \tag{3}$$

In particular, the ground state energy only depends on the interaction potential V through its scattering length $\mathfrak{a}$.

Moreover, in [7, 15, 14], it was later shown that any normalized sequence $\psi_N \in L^2_s(\Lambda^N)$ of approximate ground states of the Hamiltonian H_N with

$$\frac{1}{N}\langle \psi_N, H_N \psi_N \rangle \to 4\pi\mathfrak{a},$$

exhibits *complete* Bose–Einstein condensation in the zero-momentum state $\phi_0 \equiv 1$, in the sense that the corresponding one-particle reduced density matrix γ_N (normalized so that Tr $\gamma_N = 1$) satisfies

$$\lim_{N\to\infty} \langle \phi_0, \gamma_N \phi_0 \rangle = 1. \tag{4}$$

Recently, there has been some progress in the rigorous understanding of the spectral properties of interacting Bose gases in the Gross–Pitaevskii limit, beyond the leading order estimates (3) and (4). These results were first proved in [3, 6, 4] and are based on a rigorous version of Bogoliubov theory. They can be summarized as follows.

Theorem 1. *Let $V \in L^2(\mathbb{R}^3)$ be non-negative, radial and compactly supported.*

(i) Optimal rate for condensation: *Let $\psi_N \in L^2_s(\Lambda^N)$ be a sequence of approximate ground states such that for all*

$$\langle \psi_N, H_N \psi_N \rangle \leq 4\pi\mathfrak{a}N + K \tag{5}$$

for some $K > 0$. Then there exists a constant $C > 0$ such that for all $N \in \mathbb{N}$

$$1 - \langle \phi_0, \gamma_n \phi_0 \rangle \leq \frac{C(K+1)}{N}. \tag{6}$$

(ii) Precise estimate for the ground state energy: *For $N \in \mathbb{N}$ we have*

$$\begin{aligned} E_N(V) =& 4\pi\mathfrak{a}(N-1) + e_\Lambda \mathfrak{a}^2 + \frac{1}{2}\sum_{p \neq 0}\Bigg(\sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - p^2 \\ & - 8\pi\mathfrak{a} + \frac{(8\pi\mathfrak{a})^2}{2p^2}\Bigg) + \mathcal{O}(N^{-1/17}), \end{aligned} \tag{7}$$

where

$$e_\Lambda := 2 - \lim_{M\to\infty} \sum_{p \in \mathbb{Z}^3 \setminus \{0\} : ||p||_\infty \leq M} \frac{\cos(|p|)}{p^2}$$

and, in particular, this limit exists.

(iii) Excitation spectrum: *The spectrum of $H_N - E_N$ below a threshold $\theta \leq N^{1/17}$ consists of eigenvalues of the form*

$$\sum_{p \neq 0} n_p \sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} + \mathcal{O}(\theta N^{-1/17}) \tag{8}$$

with $n_p \in \mathbb{N}$ for all $p \in 2\pi\mathbb{Z}^3 \setminus \{0\}$.

The correction $e_\Lambda \mathfrak{a}^2$ that appears in (7) is a finite volume effect and arises because the scattering length $\mathfrak{a}$ is defined in terms of the scattering equation on the whole space $\mathbb{R}^3$, rather than on the unit torus Λ, cf. (2). The precise form of the correction was first calculated in [6].

Alternatively, this correction can also be captured by considering the so-called *box scattering length* which for $N \in \mathbb{N}$ is defined by

$$8\pi\mathfrak{a}_N := \hat{V}(0) + N\sum_{p \neq 0} \hat{V}_N(p)\varphi_p, \tag{9}$$

where

$$\hat{V}_N(r) = \frac{1}{N}\hat{V}(r/N)$$

and the coefficients $(\varphi_p)_{p \in 2\pi\mathbb{Z}^3 \setminus \{0\}}$ solve the equations

$$p^2 \varphi_p + \frac{1}{2}\sum_{q \neq 0} \hat{V}_N((p-q))\varphi_q = -\frac{1}{2}\hat{V}_N(p).$$

for every $p \in 2\pi\mathbb{Z}^3 \setminus \{0\}$. One can then show that satisfies $|\mathfrak{a}_N - \mathfrak{a}| \lesssim N^{-1}$ and gets the following alternative expression for the ground state energy:

$$
\begin{aligned}
E_N(V) = & 4\pi\mathfrak{a}_N(N-1) + \frac{1}{2}\sum_{p\neq 0}\left(\sqrt{|p|^4 + 16\pi\mathfrak{a}p^2} - p^2 - 8\pi\mathfrak{a} + \frac{(8\pi\mathfrak{a})^2}{2p^2}\right) \\
& + \mathcal{O}(N^{-1/17}),
\end{aligned} \tag{10}
$$

Analogous results have also been established for Bose gases trapped by external potentials in the Gross–Pitaevskii regime [19, 20, 21, 22] and for scaling regimes interpolating between the Gross–Pitaevskii regime and the thermodynamic limit, see [17, 18].

To outline the proof of Theorem 1 we follow [5]. It is convenient to switch to second quantization. For momenta $p \in \Lambda^* = 2\pi\mathbb{Z}^3$ let $u_p(x) = e^{ip\cdot x}$ and define the annihilation operators $a_p = a(u_p)$. In terms of creation and annihilation operators the Hamiltonian (1) becomes

$$
H_N = \sum_{p\in\Lambda^*} p^2 a_p^\dagger a_p + \frac{1}{2}\sum_{r,p,q\in\Lambda^*} \hat{V}_N(r) a_{p+r}^\dagger a_q^\dagger a_p a_{q+r}.
$$

Compared to the mean-field regime, the interaction V_N decays slowly in momentum space.

Prior results [7, 14] show the condensation of low energy states in the zero momentum state. The intuition therefore is that, for low energy states $\mathcal{N}_+ = \sum_{p\neq 0} a_p^\dagger a_p$ should be much smaller than N and therefore $N \approx \mathcal{N}_0 = a_0^\dagger a_0$. Since $[a_0, a_0^\dagger] = 1 \ll N$, both a_0 and $a_0^\dagger$ appear to be of order $\sqrt{N}$. This motivates separating the Hamiltonian into several terms according to the number of zero momentum creation and annihilation operators appearing. For the term with all four momenta equal to zero, one uses that

$$
a_0^\dagger a_0^\dagger a_0 a_0 = \mathcal{N}_0(\mathcal{N}_0 - 1) = N(N-1) - \mathcal{N}_+(2N-1) + \mathcal{N}_+^2
$$

and combines the last two terms with the terms with two zero momenta. This gives

$$
H_N = H_0 + H_1 + H_2 + Q_2 + Q_3 + Q_4
$$

where

$$
\begin{aligned}
H_0 &= \hat{V}_N(0)\frac{N(N-1)}{2}, \qquad H_1 = \sum_{p\neq 0} p^2 a_p^\dagger a_p, \\
H_2 &= \sum_{p\neq 0} \hat{V}_N(p) a_p^\dagger a_p (N - \mathcal{N}_+) - \hat{V}_N(0)\frac{\mathcal{N}_+(\mathcal{N}_+ - 1)}{2},
\end{aligned}
$$

and

$$Q_2 = \frac{1}{2}\sum_{p\neq 0} \hat{V}_N(p)[a_p^\dagger a_{-p}^\dagger a_0 a_0 + \text{h.c.}]$$
$$Q_3 = \sum_{q,r,q+r\neq 0} \hat{V}_N(r)[a_{q+r}^\dagger a_{-r}^\dagger a_q a_0 + \text{h.c.}]$$
$$Q_4 = \frac{1}{2}\sum_{p,q,r+p,r+q\neq 0} \hat{V}_N(p) a_{p+r}^\dagger a_q^\dagger a_p a_{q+r}.$$

The H-terms are (approximately) diagonal in creation and annihilation operators, while the Q-terms are off-diagonal. Counting powers, Q_3 and Q_4 seem negligible. However, in contrast to the mean-field regime, they actually give relevant contributions due to the slow decay of the interaction in momentum space, even at leading order. To find the spectrum, the strategy is to approximately diagonalize the Hamiltonian. While we follow the strategy in [5], there are other approaches to diagonalization, for instance [6, 4, 12].

The first step is to remove the big contributions hidden in Q_2 by conjugating with a suitable unitary. For this, one makes the ansatz e^{B_2} with

$$B_2 = \sum_{p\in\Lambda^*} \tilde{\varphi}_p (a_p^\dagger a_{-p}^\dagger a_0 a_0 - \text{h.c.}),$$

where $\tilde{\varphi}_p$ still has to be chosen. Note that B_2 has the same structure as for a Bogoliubov transform, just with other coefficients $\tilde{\varphi}_p$. One can rewrite

(11)
$$e^{-B_2}(H_1 + Q_2 + Q_4)e^{B_2} = H_1 + Q_2 + \int_0^1 e^{-tB_2}([H_1 + Q_4, B_2] + Q_2)e^{tB_2}\mathrm{d}t$$
$$+ \int_0^1 \int_s^1 e^{-tB_2}[Q_2, B_2]e^{tB_2}\mathrm{d}t\mathrm{d}s.$$

The idea is to choose $\tilde{\varphi}$ such that the term in the first integral approximately vanishes, which happens if $f = 1 + \tilde{\varphi}$ satisfies the scattering equation restricted to nonzero momenta. It is convenient to restrict $\tilde{\varphi}$ to high momenta $|p| > N^\alpha$ for some $0 < \alpha < 1$, as this allows to expand the exponential. As a trade-off in the integral there is still a term $\tilde{Q}_2$ of the form $a_p^\dagger a_{-p}^\dagger \frac{a_0 a_0}{N}$ left for low momenta. The integral can be rewritten as

(12)
$$\int_0^1 e^{-tB_2}\tilde{Q}_2 e^{tB_2} = \tilde{Q}_2 + \int_0^1 \int_0^s e^{-tB_2}[\tilde{Q}_2, B_2]e^{tB_2}\mathrm{d}t\mathrm{d}s.$$

Conjugating the full Hamiltonian H_N and making use of the definition of $\tilde{\varphi}$ gives

$$(13)\quad \begin{aligned} e^{-B_2}H_N e^{B_2} =& 4\pi\mathfrak{a}_N(N-1) + \sum_{p\neq 0}(p^2 + 2\hat{V}(0) - 8\pi\mathfrak{a}_N)a_p^\dagger a_p \\ &+ \sum_{0\neq|p|<N^\alpha} 4\pi\mathfrak{a}_N(a_p^\dagger a_{-p}^\dagger \frac{a_0 a_0}{N} + \text{h.c.}) + \frac{1}{4}\sum_{0\neq|p|<N^\alpha}\frac{(8\pi\mathfrak{a}_N)^2}{p^2} \\ &+ Q_3 + Q_4 + \text{error}. \end{aligned}$$

In particular, the leading order is correct now, due to a contribution coming from the last term in (11), which also contributes the $\hat{V}(0) - 8\pi\mathfrak{a}_N$ to the second term. The second $\hat{V}(0)$ stems from H_2. The third term is essentially $\tilde{Q}_2$. The fourth term stems from combining the last term in (11) with the last term in (12) using the scattering equation. The Q_3 term is not affected significantly by conjugation. The error terms consist of operators that turn out to be small on low-energy states.

Similarly, to remove Q_3 next, B_3 is chosen such that $[H_1 + Q_4, B_3] + Q_3 \approx 0$, which leads to the choice $B_3 = \sum_{p,q}\tilde{\varphi}_p \chi_{|q|<N^\alpha} a_{p+q}^\dagger a_{-p}^\dagger a_q a_0$. Conjugation with e^{B_3} effectively removes Q_3 and replaces $\hat{V}(0)$ by $8\pi\mathfrak{a}_N$ in (13). Then, if we ignore Q_4 and recall that $a_p^\dagger a_p \approx a_p^\dagger \frac{a_0 a_0^\dagger}{N} a_p$ the remaining Hamiltonian is essentially quadratic in the operators $b_p := \frac{a_0^\dagger}{\sqrt{N}} a_p$, which satisfy approximate bosonic commutation relations. Motivated by the standard Bogoliubov transform, one conjugates with e^{B_4} where $B_4 = \frac{1}{2}\sum_{0\neq|p|<N^\alpha}\tau_p(b_p^\dagger b_{-p}^\dagger - \text{h.c.})$ with $\tau_p = -1/4\log(1 + 16\pi\mathfrak{a}_N/p^2)$. Denoting $U = e^{B_2}e^{B_3}e^{B_4}$ one obtains

$$(14)\quad \begin{aligned} U^\dagger H_N U = 4\pi\mathfrak{a}_N(N-1) &+ \sum_{p\neq 0}\left(\sqrt{p^4 + 16\pi\mathfrak{a}_N p^2} - p^2 - 8\pi\mathfrak{a}_N + \frac{(8\pi\mathfrak{a}_N)^2}{2p^2}\right) \\ &+ \sum_{p\neq 0}\sqrt{p^4 + 16\pi\mathfrak{a}_N p^2}\, a_p^\dagger a_p + e^{-B_4}Q_4 e^{B_4} + \text{error} \end{aligned}$$

The error terms contain the operators H_1, Q_4 and powers of $\mathcal{N}_+$.

Proof ideas for i in Theorem 1. Note that in the language of the second quantisation, it suffices to show that on the sector $\{\mathcal{N} = N\}$, we have

$$(15)\quad H_N \geq 4\pi\mathfrak{a}_N N + C^{-1}\mathcal{N}_+ - C$$

for some constant $C > 0$ independent of N. The proof of (15) combines the representation obtained in (14) with a *localization in the number of particles* argument. To sketch the main idea behind this, let $f, g : \mathbb{R} \to [0,1]$ be smooth functions such that $f(s)^2 + g(s)^2 = 1$ for all $s \in \mathbb{R}$, $f(s) = 1$ for $s \leq 1/2$ and $f(s) = 0$ for $s \geq 1$. For $M_0 > 0$ we define $f_{M_0} = f(\mathcal{N}_+/M_0)$ and $g_{M_0} = g(\mathcal{N}_+/M_0)$. Then we can write

$$(16)\quad H_N = f_{M_0}H_N f_{M_0} + g_{M_0}H_N g_{M_0} + \mathcal{E}_{M_0}$$

with error term given by

$$\mathcal{E}_{M_0} = \frac{1}{2}\left([f_{M_0}, [f_{M_0}, H_N]] + [g_{M_0}, [g_{M_0}, H_N]]\right).$$

Choosing $M_0 = \varepsilon N$, for $\varepsilon > 0$ to be fixed later, one can then estimate the three terms appearing in (16) separately. The first term corresponds to the case where we have few excitations, i.e., $\mathcal{N}_+ \le \varepsilon N$, so the representation and bound for the error term in (14) allow us to conclude

$$f_{M_0} H_N f_{M_0} \ge f_{M_0}^2 (4\pi \mathfrak{a}_N N + C_1^{-1}\mathcal{N}_+ - C_1)$$

for some $C_1 > 0$ independent of N. For the second term in (16), corresponding to the case where there are many excitations, i.e., $\mathcal{N}_+ \ge \frac{\varepsilon}{2}N$ one can argue by contradiction. If there was no constant C_2 such that

$$g_{M_0}(H_N - 4\pi\mathfrak{a}_N N) g_{M_0} \ge C_2^{-1}\mathcal{N}_+ g_{M_0}^2, \tag{17}$$

then one could construct a normalised sequence Ψ_N satisfying

$$\left|\frac{1}{N}\langle \Psi_N, H_N \Psi_N\rangle - 4\pi\mathfrak{a}_N\right| \to 0$$

on the one hand and being supported on $\{\mathcal{N}_+ > \frac{\varepsilon}{2}N\}$ on the other hand. This contradicts (4) and allows us to conclude that (17) holds for some constant $C_2 > 0$ independent of N. Finally, one can use the canonical commutation relations to suitably rewrite the commutators for $h = f, g$ in the error term $\mathcal{E}_{M_0}$ into a form that can then be estimated by applying Taylor's formula to the smooth functions f, g.

Proof ideas for parts *ii* and *iii* of Theorem 1. Let G_N denote the right hand side of (14) without the Q_4 and the error term. Since $\mathfrak{a}_N \approx \mathfrak{a} + O(1/N)$, G_N has exactly the ground state energy stated in (10) and the excitation spectrum as in part *iii* of Theorem 1. The eigenstates are of the form

$$\xi = \prod_{j=1}^{k} \frac{a^\dagger(p_j)^{n_j}}{\sqrt{n_j!}}\Omega$$

where Ω denotes the vacuum. To prove the theorem, one has to show that for all $0 < \theta < N^{1/17}$ the L-th eigenvalue $\lambda_L(H_N) = \lambda_L(G_N) + O(\theta N^{-1/17})$ for all L with $\lambda_L(H_N) < \theta$. To show $\lambda_L(H_N) \ge \lambda_L(G_N) + O(\theta N^{-1/17})$ the key ingredients are localization in the number of particles and positivity of Q_4. To show that $\lambda_L(H_N) \le \lambda_L(G_N) + O(\theta N^{-1/17})$ one needs to bound $e^{-B_4} Q_4 e^{B_4}$ + error on the space spanned by the first L eigenstates of G_N. Using the explicit form of the eigenstates of G_N, one can bound the Q_4 term (in contrast, Q_4 was large on low energy states of H_N.) To handle error terms, condensation at optimal rate and Gronwall arguments are used.

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Heuristic derivation of the Lee-Yuang-Hang formula and the energy of quasi free states

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We consider a system of N identical bosons in the box $\Lambda = [-L/2, L/2] \subset \mathbb{R}^3$ with periodic boundary conditions. The Hamiltonian is

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i}) + \frac{1}{2}\sum_{i\neq j=1}^{N} V(x_i - x_j), \tag{1}$$

where V is a periodization of a radially symmetric potential V_∞ defined on $\mathbb{R}^3$. Since the particles are bosons, H_N acts on the symmetric subspace $L^2_{\mathrm{sym}}(\Lambda^N) \subset L^2(\Lambda^N)$. The thermodynamic (infinite volume) ground state energy density is

$$e(\rho) = \lim_{\substack{L\to\infty \\ \frac{N}{L^3}\to\rho}} \frac{E_L(N)}{L^3}, \qquad \text{where } E_L(N) = \inf_{\psi\in L^2_{\mathrm{sym}}(\mathbb{R}^3)} \frac{\langle\psi, H_N\psi\rangle}{\langle\psi,\psi\rangle}. \tag{2}$$

In 1957 [7], Lee, Huang and Yang conjectured that in the dilute limit $\rho a^3 \to 0$,

$$e(\rho) = 4\pi\rho^2 a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o(\sqrt{\rho a^3})\right) \tag{3}$$

Remarkably, this formula shows that the first two terms of the ground state energy expansion depend on the interaction potential only through the scattering length a, which characterizes its effective range. Their derivation, based on the pseudo-potential method, provided deep physical insight but lacked mathematical rigor. A later, still non-rigorous, approach was proposed in [8]. Establishing the Lee-Huang-Yang (LHY) formula rigorously has proved challenging: Dyson [3] first obtained the correct leading-order upper bound, later matched by Lieb and Yngvason [10] for all positive potentials with finite scattering length, including hard-core interactions. The LHY correction in the translation-invariant thermodynamic setting was first proved as an upper bound for smooth, rapidly decaying potentials by Yau and Yin [14], then extended to a broader class in [1] by Basti, Cenatiempo and Schlein, with the corresponding lower bound, including hard-core cases, finally established in [5, 6] by Forunais and Solovej.

We now present a heuristic derivation of the LHY formula, following [9], starting from Bogoliubov's seminal theory [2]. We switch to the second-quantized formalism with Fock space $\mathcal{F} = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\Lambda^n)$ and creation/annihilation operators a_k^* and a_k. The essence of Bogoliubov's approach is to work in momentum space, where the Hamiltonian reads

$$\mathcal{H} = \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} |k|^2 a_k^* a_k + \frac{1}{2L^3}\sum_{k,q,p\in\frac{2\pi}{L}\mathbb{Z}^3} \hat{V}(p) a^*_{k+p} a^*_{q-p} a_q a_k,$$

with $\hat{V}(p) = \int_\Lambda dx\, V(x) e^{ip\cdot x}$.

In his 1947 paper [2], Bogoliubov introduced an approximate model (now known as the Bogoliubov approximation) for weakly interacting Bose gases. To motivate this approximation, consider first the non-interacting case, where the ground state is[1] $(N!)^{1/2}(a_0^*)^N|\Omega\rangle$ with all particles occupying the zero momentum mode (the condensed state). When interactions are turned on, V couples pairs of particles with momenta p and q to $p+k$ and $q-k$. Expecting Bose-Einstein condensation, the zero momentum mode ($p=0$) plays a special role: starting from the fully condensed state, interactions primarly create pairs with opposite momenta k and $-k$, as well as higher-order excitations. Assuming a weak interactions, one expects that most particles remain in the condensate, i.e., that N_0/N is still a number of order unity (condensation hypothesis) and that the remaining fractions are largely grouped into pairs. This underlies Bogoliubov's approximation: retain in the Hamiltonian $\mathcal{H}$ only terms involving either[2] two or four particles zero momentum particles, neglecting all others. Furthermore, based on the condensation hypothesis, Bogoliubov suggested to replace a_0, a_0^* by $\sqrt{N_0} \simeq \sqrt{N}$. The resulting quadratic Hamiltonian is

$$H_{\mathrm{Bog}} = \frac{1}{2}N\rho\hat{V}(0) + \sum_{k\in\Lambda^*}\left(|k|^2 + \rho\hat{V}(k)\right)a_k^*a_k + \frac{1}{2}\sum_{k\in\Lambda^*}\rho\hat{V}(k)\left(a_ka_{-k} + a_{-k}^*a_k^*\right), \tag{4}$$

where $\Lambda^* = (2\pi/L)\mathbb{Z}^3 \setminus \{0\}$. Being quadratic, H_{Bog} can be diagonalized via a Bogoliubov transformation. In our setting, this transformation can be written as $T = e^{iS}$, with

$$iS = \frac{1}{2}\sum_{k\in\Lambda^*}\varphi(k)\left(a_k^*a_{-k}^* - \mathrm{h.c.}\right),$$

so that $a_k \to b_k = e^{iS}a_ke^{-iS} = a_k\cosh\varphi(k) - a_{-k}^*\sinh\varphi(k)$.
Choosing $\tanh 2\varphi(k) = \rho\hat{V}(k)/(|k|^2 + \rho\hat{V}(k))$, we obtain[3]

$$\begin{aligned} H_{\mathrm{Bog}} \to H'_{\mathrm{Bog}} = &\frac{N}{2}\rho\hat{V}(0) - \frac{1}{2}\sum_{k\in\Lambda^*}(|k|^2 + \rho\hat{V}(k)) - \sqrt{(|k|^2 + \rho\hat{V}(k))^2 - \rho^2|\hat{V}(k)|^2} \\ &+ \sum_{k\in\Lambda^*}\sqrt{|k|^2 + 2|k|\rho\hat{V}(k))}b_k^*b_k. \end{aligned} \tag{5}$$

The last term gives the excitation spectrum, linear in k for small k, a key feature underlying superfluidity. The ground state wave function is the vacuum of the b's operators appearing in (4), giving the energy density

$$e(\rho) = \frac{\rho^2\hat{V}(0)}{2} - \frac{1}{2}\int_0^\infty dk\,\left\{|k|^2 + \rho\hat{V}(k) - \sqrt{|k|^2 + 2|k|\rho\hat{V}(k)}\right\}.$$

Bogoliubov thus obtains that the leading contribution in the energy expansion gives the zeroth-order term in the Born series for the scattering length (see e.g., [4, Lemma 3] for details). Following [9], and aiming to recover (3), we add and substract the next Born term, $-\int dp\,|\hat{V}(p)|^2/(2|p|^2)$ multiplied by $\rho^2/2$, yielding

$$e(\rho) = 4\pi\rho^2(a_0+a_1) - \frac{1}{2}\int_0^\infty dk\,\left\{|k|^2 + \rho\hat{V}(k) - \sqrt{|k|^2 + 2|k|\rho\hat{V}(k)} - \frac{\rho^2|\hat{V}(p)|^2}{2|p|^2}\right\}, \tag{6}$$

[1] Here Ω denotes the vacuum state in $\mathcal{F}$.

[2] Note that the case of 3 momenta equal to 0 and one not is not allowed by momentum conservation.

[3] The transformation is well defined provided $|k|^2 + \rho\hat{V}(k) > 0$, which holds for repulsive or weakly attractive $\hat{V}(k)$.

with $a_0 = \hat{V}(0)/8\pi a$ and $a_1 = (8\pi)^{-1} \int dp\, |\hat{V}(p)|^2/(2|p|^2)$. For smooth $\hat{V}(k) \to 0$ vanishing faster than $|k|^{-1}$ at infinity, the integral above contributes only for small $|k|$. Thus, assuming further that $\hat{V}(0) \neq 0$, we replace $\hat{V}(k)$ by $\hat{V}(0)$ in the integrand. After rescaling, the integral in (6) is $\mathcal{O}(\rho^{5/2})$, giving

$$e(\rho) = 4\pi\rho^2(a_0 + a_1) + 4\pi a_0 \rho^2 (\rho a_0^3)^{\frac{1}{2}} \frac{128}{15\sqrt{\pi}}. \tag{7}$$

This concludes the heuristic derivation of the LHY formula. However, comparing (7) with (3), the first Born terms should be replaced by the full scattering length. A natural first step toward this is to consider the energy of quasi-free states, since the Bogoliubov approximation replaces the Hamiltonian with a quadratic one, whose ground state is quasi-free. Restricting to pure states, a quasi-free state is obtained by a Bogoliubov transformation on the Fock vacuum Ω. Before proceeding further, let us take a step back and recall that the substitution $a_0^*, a_0 \mapsto \sqrt{N_0} \simeq \sqrt{N}$ can be rigorously implemented via a Weyl transformation

$$W_0 = \exp\left(\sqrt{N_0} a_0^* - \sqrt{N_0} a_0\right),$$

which acts on the creation operators as $W_0^* a_0^* W_0 = a_0^* + \sqrt{N_0}$ and $W_0^* a_k^* W_0 = a_k^*$ for any $k \neq 0$, and analogously on the annihilation operators. Conjugating $\mathcal{H}$ by W_0 rewrites the Hamiltonian in terms of fluctuations around the condensate of density $\rho_0 = N_0/L^3$ in the zero momentum state. Evaluating the energy in the coherent state $W_0\Omega$ fails to reproduce the correct energy even at leading order. A better approximation is obtained by evaluating $W_0^* \mathcal{H} W_0$ in a translation invariant quasi-free state, where all expectation values can be expressed via Wick's Theorem in terms of

$$\gamma(k) = \langle a_k^* a_k \rangle, \qquad \alpha(k) = \langle a_k^* a_{-k}^* \rangle, \qquad \text{with} \quad \alpha^2(k) \leq \gamma(k)(1 + \gamma(k)))$$

In the thermodynamic limit, the energy density of such a state is given by

$$\begin{aligned} &\frac{1}{2}\hat{V}(0)\left(\rho_0 + \frac{1}{(2\pi)^3}\int dp\, \gamma(p)\right)^2 + \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} dp\, p^2 \gamma(p) \\ &+ \frac{\rho_0}{(2\pi)^3}\int dp\, \hat{V}(p)\,(\gamma(p) + \alpha(p)) + \frac{1}{2(2\pi)^6}\int dp dq\, \hat{V}(p-q)(\gamma(p)\gamma(q) + \alpha(p)\alpha(q)). \end{aligned} \tag{8}$$

Comparing this expression with the Bogoliubov Hamiltonian (4), we see that Bogoliubov neglects the last term in (8), arising from the interaction involving four nonzero momenta $\hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p$. This contribution is crucial to recover the correct scattering length dependence of the energy. Indeed, [4] showed that, evaluating the full Hamiltonian on quasi-free states reproduces the leading term at the level of the upper bound

$$e(\rho) \leq 4\pi a \rho^2 (1 + \mathcal{O}((\rho a^3)^{1/2}),$$

and that the full LHY upper bound can be obtained for potentials of the form $V(x) = \lambda \widetilde{V}(x)$, with $\lambda > 0$ sufficiently small, and $\widetilde{V}$ non-negative, smooth, radially symmetric and with suitable decay decay. Quasi-free states have also been studied at positive temperature [11, 12]; see also the discussion in [13]. While capturing the leading order, they fail to include quantum correlations necessary for the LHY term; a deeper analysis is thus required to recover the complete LHY formula (3).

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Free Energy of Dilute Bose Gas at Low Temperature: Lower Bound

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We estimate the free energy of a dilute Bose gas at low temperature following [2] and focusing on a rigorous lower bound consistent with the Lee–Huang–Yang (LHY) correction. The technique of Neumann bracketing is presented, and a crucial cubic renormalization justifies the appearance of the scattering length of the interaction in the expansion.

We set the centered box of length ℓ to be $\Lambda_\ell := [-\frac{\ell}{2}, \frac{\ell}{2}]^3$ and consider the Hamiltonian of a many–body bosonic system given by

$$\mathcal{H}_{n,\ell} := \sum_{i=1}^{n}(-\Delta_{x_i}) + \sum_{1\le i<j\le n} V(x_i - x_j)$$

on $L^2_s(\Lambda_\ell^n)$, where the interaction kernel V is chosen to be nice enough and have scattering length a, that is, if w is the solution to the scattering equation $\Delta w = V(1-w)$, $a := \int_{\mathbb{R}^3} V(1-w)$. Rescaling the Hamiltonian by conjugating with the map $U : \Psi \mapsto \ell^{\frac{3}{2}}\Psi(\ell\cdot)$, we derive the following rescaled many–body Hamiltonian on the unit box $L^2_s(\Lambda^n)$

$$U^*\mathcal{H}_{n,\ell}U := \frac{1}{\ell^2}\left[\sum_{i=1}^{n}(-\Delta_{x_i}) + \sum_{1\le i<j\le n} V_\ell(x_i - x_j)\right] =: \frac{1}{\ell^2}\tilde{\mathcal{H}}_{n,\ell}, \tag{1}$$

where we denote the rescaled interaction as $V_\ell := \ell^2 V(\ell\cdot)$ and abbreviate $\Lambda = \Lambda_1$. As predicted in the seminal work by Lee, Huang and Yang [1], we aim at proving (under suitable unitary transform)

$$\tilde{\mathcal{H}}_{n,\ell} \cong 4\pi a n\frac{n}{\ell} + 4\pi\frac{128}{15\sqrt{\pi}}a^{\frac{5}{2}}\left(\frac{n}{\ell}\right)^{\frac{5}{2}} + \mathrm{d}\Gamma\left(\sqrt{p^4 + 8\pi a\frac{n}{\ell}p^2}\right) + \text{l.o.t.} \tag{2}$$

for some well-chosen scale ℓ.

Remark 1. The Neumann boundary condition is imposed, as the merit of using such boundary condition for lower bound can already be witnessed in Dyson's lemma. In [2], the length scale is chosen slightly larger than the Gross–Pitaevskii length scale. The reason is that on one hand, as the proof of BEC in the hydrodynamic limit is still a major open problem in the field, the length scale cannot be chosen to be too large; while on the other hand, the spectral gap of the kinetic energy balances with the interaction energy, which poses significant challenges for controlling Neumann boundary effects.

Remark 2. As alluded to by the title, the asymptotic expansion should lead to the lower bound of the free energy at low temperature ($0 \le T \le \rho a \cdot (\rho a^3)^{-\kappa}$ for small $\kappa > 0$, where ρ is the particle density)

$$\begin{aligned}-T\log\mathrm{Tr}\left[\exp\left(-\frac{\tilde{\mathcal{H}}_{n,\ell}}{T\ell^2}\right)\right] =: F_\ell(n) \ge 4\pi\frac{a}{\ell^3}n^2\left[1 + \frac{128}{15\sqrt{\pi}}n^{\frac{1}{2}}\left(\frac{a}{\ell}\right)^{\frac{3}{2}}\right]\\ + T\sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\log\left[1 - \exp\left(-\frac{1}{T\ell^2}\sqrt{p^4 + 16\pi a\frac{n}{\ell}p^2}\right)\right] + \text{l.o.t.},\end{aligned} \tag{3}$$

for $n \lesssim \rho\ell^3$, which, together with the sub–additivity of the free energy and the chemical potential (forcing $\frac{n}{\ell^3} \sim \rho$ in small boxes) further imply the lower bound of free energy in the hydrodynamic limit, namely in the dilute limit,

$$\begin{aligned}\lim_{\substack{N\to\infty\\ N/L^3\to\rho}}\frac{F_L(N)}{L^3} \ge 4\pi a\rho^2\left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3}\right]\\ + \frac{T^{\frac{5}{2}}}{(2\pi)^3}\int_{\mathbb{R}^3}\log\left[1 - \exp\left(-\sqrt{p^4 + \frac{16\pi\rho a}{T}p^2}\right)\right]\mathrm{d}p + \text{l.o.t.}\end{aligned} \tag{4}$$

The derivation of the above estimates from (2) is very involved, so we refer the readers to the original works and focus only on the informal derivation of (2) itself.

Neumann Boundary

We set the truncated scattering solution $w_{\ell,\lambda} := w(\ell\cdot)\chi_\lambda$, where χ_λ is a smooth cutoff function supported on the centered ball of radius λ chosen properly, and we define

$$\frac{1}{2}\epsilon_{\ell,\lambda} := \Delta w_{\ell,\lambda} + \frac{1}{2}V_\ell(1-w_\ell) \Rightarrow \int_{\mathbb{R}^3}\epsilon_{\ell,\lambda} = \int_{\mathbb{R}^3}\frac{1}{2}V_\ell(1-w_\ell) = \frac{8\pi a}{\ell}. \tag{5}$$

The reason for introducing the truncation χ_λ is that w_ℓ is harmonic outside a centered ball and therefore can not be periodized directly. For Neumann boundary conditions, we consider the basis $\{u_p\}_{p\in\pi\mathbb{N}_0^3}$ where $u_p(x) := \prod_{k=1}^3 \sqrt{2}\cos(p_i(x_i + \frac{1}{2}))$, and construct the kernel K as

$$K(x,y) := -\sum_{z\in\mathbb{Z}^3} n w_{\ell,\lambda}(P_z(x)-y) - n\hat{w}_{\ell,\lambda}(0), \tag{6}$$

where P_z is the mirroring transform and we refer to (1.21) in [2] for details. It can be shown directly from the construction that

Proposition 3. *The kernel K is diagonal under the Neumann basis, that is*

$$K = -\sum_{p\in\pi\mathbb{N}_0^3\backslash\{0\}} n\hat{w}_{\ell,\lambda}(p)u_p^{\otimes 2}, \tag{7}$$

and further

$$\left| n\hat{V}_\ell(0) + \int_{\Lambda^2} V_\ell(x-y)K(x,y)\mathrm{d}x\mathrm{d}y - 8\pi a\frac{n}{\ell}\right| \lesssim \frac{n\log(\ell)}{\ell^2}. \tag{8}$$

We remark that leading term inside the norm in (8) is of order $\frac{n}{\ell}$, so we almost gain $\frac{1}{\ell}$. It is also due to (8) that we correct the first two orders of the Born approximations by the scattering length itself, which will be shown in the following renormalization procedures.

Renormalization Procedures

We know that after the rigorous c–number substitution $\tilde{\mathcal{H}}_{n,\ell} \cong \chi_+^{\leq n}\mathcal{H}\chi_+^{\leq n}$, where $\chi_+^{\leq n}$ is the projection onto $\mathcal{F}_+^{\leq n}$ introduced in the previous lectures, and

$$\mathcal{H} \approx \frac{n^2}{2}V_\ell^{0000} + \sum_{k=1}^4 Q_k + \mathcal{H}_2, \tag{9}$$

where V with four superscripts denotes its coordinates as multiplication operator on the two–particle spaces, and

$$(10)\quad Q_2 = \frac{n}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^* a_y^* \mathrm{d}x\mathrm{d}y + \text{h.c.},\ Q_4 = \frac{1}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^* a_y^* a_x a_y \mathrm{d}x\mathrm{d}y$$

$$(11)\quad Q_3 = \sqrt{(n-\mathcal{N}+1)_+}\int_{\Lambda^2} V_\ell(x-y)a_x^* a_y^* a_x \mathrm{d}x\mathrm{d}y + \text{h.c.}$$

$$(12)\quad \mathcal{H}_2 = n\int_{\Lambda^2} V_\ell(x-y)(a_x^* a_x + a_x^* a_y)\mathrm{d}x\mathrm{d}y - nV_\ell^{0000}\mathcal{N} - \frac{1}{2}\int_{\Lambda^2} V_\ell(x-y)a_x^* a_y^* \mathrm{d}x\mathrm{d}y\mathcal{N} + \text{h.c.}$$

We now define

$$\mathcal{B}_1 := \frac{1}{2}\int_{\mathbb{R}^3} K(x,y)a_x^* a_y^* \mathrm{d}x\mathrm{d}y - \text{h.c.} \tag{13}$$

$$\mathcal{B}_c := \frac{\theta_M(\mathcal{N})}{\sqrt{n}}\int_{\mathbb{R}^3} K(x,y)q_x^* a_y^* q_x \mathrm{d}x\mathrm{d}y - \text{h.c.} \tag{14}$$

where $\theta_M(\mathcal{N})$ is a suitable cutoff of the number operator and q_x is the modified annihilation operator which ensures that $e^{\mathcal{B}_c}$ leaves $\mathcal{F}_+$ invariant. Using the facts that

$$\frac{n^2}{2}V_\ell^{0000} + \frac{1}{2}[Q_2,\mathcal{B}_1] \approx 4\pi a n\frac{n}{\ell} \tag{15}$$

$$[\mathrm{d}\Gamma(-\Delta)+Q_4,\mathcal{B}_1] + Q_2 \approx \underbrace{\frac{n}{2}\int_{\Lambda^2}\sum_{z\in\mathbb{Z}^3}\epsilon_{\ell,\lambda}(P_z(x)-y)a_x^* a_y^* \mathrm{d}x\mathrm{d}y}_{:=\tilde{Q}_2} + \text{h.c.} + \text{boundary term}, \tag{16}$$

where (15) is essentially due to (8), while one can interpret (16) as replacing the short–range interaction with a long–range one, which we know how to deal with the mean–field case. The boundary term is also removed by the cubic renormalization. In summary, we have after the first unitary transformation that

$$e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1} \approx \frac{4\pi a n^2}{\ell} + \sum_{p\in\pi\mathbb{N}_0^3\setminus\{0\}}\frac{|n\hat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2} + \mathrm{d}\Gamma(-\Delta) + \tilde{Q}_2 + Q_3 + Q_4 \tag{17}$$

$$+ n\int_{\Lambda^2} V_\ell(x-y)(a_x^* a_x + a_x^* a_y)\mathrm{d}x\mathrm{d}y - \frac{8\pi a n\mathcal{N}}{\ell}. \tag{18}$$

We remark that the second sum above has already appeared in the Gross–Pitaevskii regime, and the term $\frac{8\pi a n\mathcal{N}}{\ell}$ has the opposite sign that we desire, but it is corrected, together with the second last term, by the cubic renormalization so that

$$e^{-\mathcal{B}_c}e^{-\mathcal{B}_1}\mathcal{H}e^{\mathcal{B}_1}e^{\mathcal{B}_c} \approx \frac{4\pi a n^2}{\ell} + \mathbb{H}_{\mathrm{Bog}} + Q_4, \tag{19}$$

where

(20)
$$\mathbb{H}_{\mathrm{Bog}} = \sum_{p\neq 0}\left(p^2 + \frac{8\pi a n}{\ell}\right) a_p^* a_p + \frac{1}{2}\sum_{p\neq 0} n\hat{\epsilon}_{\ell,\lambda}(p)\left(a_p^* a_p^* + a_p a_p\right) + \frac{1}{2}\frac{|n\hat{\epsilon}_{\ell,\lambda}(p)|^2}{2p^2}.$$

We can then use the Bogoliubov transform to diagonalize the quadratic term, and arrive at the desired expansion (2).

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Dilute Fermions; Upper bound for the Huang-Yang formula

Lukas Junge

In this talk we discussed the ground state energy of gas consisting of dilute fermions of spin one half. The Hamiltonian we assume to model such a system is the following

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

acting on the Hilbert space

(2)
$$\mathcal{H}_N = \bigwedge^N L^2(\Lambda,\mathbb{C}^2) \cong \bigoplus_{N_\uparrow + N_\downarrow = N} \bigwedge^{N_\uparrow} L^2(\Lambda,\mathbb{C}) \otimes \bigwedge^{N_\downarrow} L^2(\Lambda,\mathbb{C}) = \bigoplus_{N_\uparrow + N_\downarrow = N} \mathcal{H}_{N_\uparrow,N_\downarrow}.$$

The above decomposition commutes with the hamiltonian and we may consider the ground state energy on each of the subspaces $\mathcal{H}_{N^\uparrow,N^\downarrow}$. In this talk the main focus was the ground state energy density in the thermodynamical limit;

$$e(\rho_\uparrow,\rho_\downarrow) = \lim_{\substack{N,L\to\infty \\ \rho_\uparrow,\rho_\downarrow fixed}} \frac{1}{L^3} \inf \sigma(H_{N|\mathcal{H}_{N_\downarrow,N_\uparrow}}).$$

We then have the following result.

Theorem 1. *[Giacomelli, Hainzl, Nam, Seiringer [3, 4]] For $V \geq 0$ compactly supported radial and $V \in L^2$. We have*

$$\begin{aligned} e(\rho_\uparrow, \rho_\downarrow) = &\frac{3}{5}(6\pi^2)^{\frac{2}{3}}(\rho_\uparrow^{\frac{5}{3}} + \rho_\downarrow^{\frac{5}{3}}) + 8\pi a \rho_\uparrow \rho_\downarrow \\ &+ \frac{(8\pi a)^2}{(2\pi)^9} \int\int\int \frac{1_{|r|\leq k_{F_\uparrow}} 1_{|r'|\leq k_{F_\downarrow}} 1_{|k+r|\geq k_{F_\uparrow}} 1_{|k-r'|\geq k_{F_\downarrow}}}{\lambda_{k,r} + \lambda_{k,r'}} \\ &- \frac{1}{2k^2} dr dr' dk + o(\rho^{\frac{7}{3}}) \end{aligned} \tag{3}$$

where a is the scattering length of the potential V and $k_{F_\sigma} = (6\pi^2\rho_\sigma)^{\frac{1}{3}}$ is the radius of the fermi ball and $\lambda_{k,r} = (k+r)^2 - r^2$.

This result is very new and the techniques we present below is state of the art.

1. Techniques and Idea of proof

We will discuss the ideas for bosonization which the author learned from [6]. We consider a trial state of the form

$$\Psi = RT_1T_2\Omega \tag{4}$$

where R is the particle hole transformation around the Fermi ball. T_1 and T_2 are unitary quasi bosonic Bogoliubov transformations. T_1 and T_2 creates pairs of excitations inside the Fermi and outside equally, and we conclude $\Psi \in \mathcal{H}_{N_\downarrow, N_\uparrow}$. We will also assume (this can be rigorously verified using the explicit form of T_1 and T_2)

$$\langle T_1T_2\Omega, \mathcal{N} T_1T_2\Omega\rangle \leq N\rho^{\frac{2}{3}-\epsilon} \tag{5}$$

for some ϵ depending on small parameters. One can then verify using both the "pair"-construction of T_1 and T_2 together with (5) that in this trail state we have

$$\begin{aligned} R^*H_NR \leq &\sum_\sigma \sum_{|k|\leq k_{F_\sigma}} k^2 + \widehat{V}(0)\frac{N_\uparrow N_\downarrow}{L^3} + \sum_{k\in\Lambda^*} |k^2 - k_{F_\sigma}^2| a_k^* a_k \\ &+ \sum_{p,q,k\in\Lambda^*} \widehat{V}(k) a^*_{p+k,\uparrow} a^*_{q-k,\downarrow} a_{q,\downarrow} a_{p,\uparrow} \widehat{u}_\uparrow(p+k)\widehat{u}_\downarrow(q-k)\widehat{u}_\downarrow(q)\widehat{u}_\uparrow(p) \\ &+ \sum_{p,q,k\in\Lambda^*} \widehat{V}(k) a^*_{p+k,\uparrow} a^*_{q-k,\downarrow} a^*_{-q,\downarrow} a^*_{-p,\uparrow} \widehat{u}_\uparrow(p+k)\widehat{u}_\downarrow(q-k)\widehat{v}_\downarrow(q)\widehat{v}_\uparrow(p) + h.c \end{aligned}$$

where $\widehat{v}$ is the projection onto the Fermi ball and $\widehat{u} = 1 - \widehat{v}$. The three last terms we call H_0, Q_4 and Q_2 respectively. T_1 renormalizes $\widehat{V}(k)$ with $\widehat{Vf}(k)$ where f is zero energy scattering solution. Using bosonization this corresponds to the high momenta Bogoliubov transformation realized perhaps first in [5]. More precisely we can write

$$T_1H_0 + Q_2 + Q_4T_1^* \sim H_0 + \tilde{Q}_2 + \frac{N_\uparrow N_\downarrow}{L^3}\widehat{Vf(1-f)}(0) - \frac{N_\uparrow N_\downarrow}{L^3}\widehat{V(1-f)}(0) \tag{6}$$

where $\tilde{Q}_2$ is the same as the previous but with $\widehat{V}(k)$ replaced with $\widehat{Vf}(k)$. For a slightly different perspective than what appears in [3] we can consider the quasi bosonic operator

$$C_{k,r,r'} = a_{p+k,\uparrow}a_{q-k,\downarrow}a_{-q,\downarrow}a_{-p,\uparrow}\widehat{u}_\uparrow(p+k)\widehat{u}_\downarrow(q-k)\widehat{v}_\downarrow(q)\widehat{v}_\uparrow(p).$$

Then one easily computes

$$[H_0, C^*_{k,r,r'}] = ((k+r)^2 - r^2 + (k-r')^2 - r'^2)C^*_{k,r,r'}$$

that implies

$$H_0 \sim \sum_{k,r,r'} \lambda_{k,r,r'} C^*_{k,r,r'} C_{k,r,r'},$$

and $\tilde{Q}_2$ is by construction linear in C. Thus, the Weyl transform

$$T_2 C_{k,r,r'} T_2^* = C_{k,r,r'} + \frac{\widehat{Vf}(k)}{L^3 \lambda_{k,r,r'}} \tag{7}$$

diagonalises the effective hamiltonian, and the constant term appearing from this diagonalization together with (6) yields Theorem 1.

2. Outlook and open problems

The straightforward question one can ask after a three term energy expansion is; “what about a four term energy expansion?”. The fourth order term has been discussed in multiple physics texts also with some discrepancies. The one presented here comes from [2] which also aligns with [1], we collect it here in full details in this notation as it might be enlightening for some.

$$e(\rho,\rho) = \mathcal{E}_1\mathcal{E}_2 + \mathcal{E}_3 + \mathcal{E}_4 + \mathcal{E}_5.$$

Here $\mathcal{E}_1$ is the two body scattering term

$$\mathcal{E}_1 = \frac{4}{3\pi}\rho k_F^3 a + \frac{1}{10\pi} k_F^5 a^2 r_0 + k_F^5 a_p^3$$

where r_0 is the so called “effective range” of v and a_p is the p-wave scattering length. All the other terms are predicted only to depend on the s-wave scattering length a. $\mathcal{E}_2$ is the Huang-Yang term;

$$\mathcal{E}_2 = \frac{(8\pi a)^2}{(2\pi)^9} \int\int\int \frac{1_{|r|\le k_F} 1_{|r'|\le k_F}(1 - 1_{|k+r|\ge k_F} 1_{|k-r'|\ge k_F})}{\lambda_{k,r} + \lambda_{k,r'}} dr dr' dk.$$

Lastly $\mathcal{E}_3, \mathcal{E}_4$ and $\mathcal{E}_5$ has the following structure

$$\mathcal{E}_3 = \frac{(8\pi a)^3}{(2\pi)^{12}} \int_{|r|\le k_F}\int_{|r'|\le k_F} \left(\int \frac{(1 - 1_{|k+r|\ge k_F} 1_{|k-r'|\ge k_F})}{\lambda_{k,r} + \lambda_{k,r'}} dk\right)^2 dr dr'$$

$$\mathcal{E}_4 = -\frac{(8\pi a)^3}{(2\pi)^{12}} \int_{|k|\ge k_F}\int_{|k'|\ge k_F} \left(\int \frac{1_{|p+k|\le k_F} 1_{|p+k'|\le k_F}}{\lambda_{k-p,p} + \lambda_{k'-p,p}} dp\right)^2 dk dk'$$

$$\mathcal{E}_5 = \frac{2(8\pi a)^3}{(2\pi)^{12}} \int_{|k|\ge k_F}\int_{|r|\le k_F} \left(\int \frac{1_{|r'+k|\ge k_F} 1_{||r'+r|\le k_F}}{\lambda_{k-r,r} + \lambda_{k+r'-r,r'-r}} dr'\right)^2 dr dk.$$

Some slightly less ambitious questions could surround the understanding of the ground state Ψ. Could something like (5) hold for the true ground state? Perhaps it hold after appropriate unitaries resembling T_1 and T_2. Is there any change this quasi bosonic picture is correct beyond the first eigenvalue, with a quasi bosonic excitation spectrum? Potentially only in a "correct" scaling regime.

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The Huang-Yang Fomula: Lower Bound

Davide Desio

In 1957, Huang and Yang predicted the ground state formula per unit volume in the thermodynamic limit for a system of spin-$\frac{1}{2}$ fermionic hard spheres having diameter $a > 0$ and spin densities $\rho_\uparrow = \rho/2 = \rho_\downarrow$. The general idea was to replace the interaction amongst particles with boundary conditions that could be rephrased in terms of a pseudopotential. Until then, the pseudopotential method had always been used for Born approximations in scattering theory. However, throughout the application of such method to the N-body hard spheres problem, they predicted the ground state energy density in the low density regime to be

$$(1)\quad e(\rho/2,\rho/2) = \frac{3}{5}(3\pi^2)^{\frac{2}{3}}\rho^{\frac{5}{3}} + 2\pi a\rho^2 + \frac{4(9\pi)^{\frac{2}{3}}}{35}(11-2\log 2)a^2\rho^{\frac{7}{3}} + o(\rho^{\frac{7}{3}})_{\rho\to 0}\ .$$

The first term in (1) may be understood as the kinetic energy of a non-interacting Fermi gas, the second term captures the leading order contribution from opposite spin interactions and the third terms comes from the renormalization of the scattering equation constrained by the Pauli blocking in the Fermi sea. A major challenge in mathematical physics is the proof of the validity of the approximation (1) from first principles. In [1], for a system with density $\rho = \rho_\uparrow + \rho_\downarrow$, it has been recently proved the upper bound

$$(2)\quad e(\rho_\uparrow,\rho_\downarrow) \leq \frac{3}{5}(6\pi^2)^{\frac{2}{3}}\left(\rho_\uparrow^{\frac{5}{3}} + \rho_\downarrow^{\frac{5}{3}}\right) + 8\pi a\rho_\uparrow\rho_\downarrow + a^2\rho_\uparrow^{\frac{7}{3}}F\left(\frac{\rho_\downarrow}{\rho_\uparrow}\right) + \mathcal{O}(\rho^{\frac{7}{3}+\frac{1}{9}})_{\rho\to 0}$$

where $F(1) = \frac{2^{2+\frac{7}{3}}(9\pi)^{\frac{2}{3}}}{35}(11-2\log 2)$ in agreement with the Huang-Yang conjecture (1). In the following, we will discuss the main ideas emploied in [2] to prove (1). First, let us define the model. We consider a spin-$\frac{1}{2}$ system of $N = N_\uparrow + N_\downarrow$ fermions in a box $\Lambda = [-L/2, L/2]^3 \subset \mathbb{R}^3$ with periodic boundary conditions. We introduce the scattering length $a > 0$ as

$$8\pi a = \int_{\mathbb{R}^3} V_\infty(x)(1-\varphi_\infty(x))\,\mathrm{d}x$$

where the interaction $V_\infty \in L^2(\mathbb{R}^3)$ is assumed to be compactly supported, radial and non-negative. The function $\varphi_\infty : \mathbb{R}^3 \to [0,1]$ is the s-wave scattering solution hence

$$\begin{cases} 2\Delta\varphi_\infty + V_\infty(1-\varphi_\infty) = 0\,, \\ \lim_{|x|\to\infty} \varphi_\infty(x) = 0\ . \end{cases}$$

Therefore, we introduce the periodization of the interaction V_∞ as

$$V(x) := \sum_{z\in\mathbb{Z}^3} V_\infty(x+zL)$$

and the N-body Hamiltonian of the system is

$$H_N := \sum_{j=1}^{N}(-\Delta_j) + \sum_{1\le i<j\le N} V(x_i - x_j)\ .$$

The second quantization of H_N on the Fock space $\mathcal{F} := \bigoplus_{n=0}^{\infty} \bigwedge^n L^2(\Lambda, \mathbb{C}^2)$ is given by

$$\mathcal{H} = \sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{k\in\mathbb{Z}^3} |k|^2 \widehat{a}^*_{k,\sigma}\widehat{a}_{k,\sigma} + \frac{1}{2}\sum_{\sigma,\sigma'\in\{\uparrow,\downarrow\}} \int_{\Lambda^2} \mathrm{d}x\,\mathrm{d}y\, V(x-y) a^*_{x,\sigma} a^*_{y,\sigma'} a_{y,\sigma'} a_{x,\sigma}\ .$$

The annihilation operator and, its adjoint, the creation operator are defined respectively as

$$\widehat{a}_{k,\sigma} = L^{-3/2}\int_\Lambda \mathrm{d}x\, e^{-ik\cdot x} a_{x,\sigma}\,, \quad \widehat{a}^*_{k,\sigma} = L^{-3/2}\int_\Lambda \mathrm{d}x\, e^{ik\cdot x} a^*_{x,\sigma}$$

where the operator valued distributions $a_{x,\sigma} = a(\delta_\sigma \delta_x)\,, a^*_{x,\sigma} = a^*(\delta_\sigma\delta_x)$ have been introduced. The ground state of the free Fermi gas is determined by filling, for any $\sigma \in \{\uparrow,\downarrow\}$, the Fermi sphere $B_F^\sigma := \{k \in \mathbb{Z}^3 : |k| \le k_F^\sigma\}$ where the Fermi radius is

$$k_F^\sigma = (6\pi^2)^{\frac{1}{3}} \rho_\sigma^{\frac{1}{3}} + o(1)_{L\to\infty}\,.$$

The Fermi sphere will be assumed to be completely filled hence $|B_F^\sigma| = N_\sigma$. This is without loss of generality since the family of ρ_σ is dense on $\mathbb{R}_+$ as $L \to \infty$.

Theorem 1 (Main Result)**.** *Let $\mathfrak{h}(N_\uparrow, N_\downarrow) \subset \bigwedge^N L^2(\Lambda, \mathbb{C}^2)$ be the subspace so that $N = N_\uparrow + N_\downarrow$. Let us define the ground state energy density as*

$$e(\rho_\uparrow,\rho_\downarrow) := \lim_{\substack{L\to\infty \\ N_\sigma/L^3\to\rho_\sigma,\sigma\in\{\uparrow,\downarrow\}}} L^{-3} \inf_{\psi\in\mathfrak{h}(N_\uparrow,N_\downarrow)} \frac{\langle\psi, H_N\psi\rangle}{\langle\psi,\psi\rangle}$$

In the limit for $\rho = \rho_\uparrow + \rho_\downarrow \to 0$, the ground state energy density satisfies:

$$e(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5}(6\pi^2)^{\frac{2}{3}} \left(\rho_\uparrow^{\frac{5}{3}} + \rho_\downarrow^{\frac{5}{3}} \right) + 8\pi a \rho_\uparrow \rho_\downarrow + a^2 \rho_\uparrow^{\frac{7}{3}} F\left(\frac{\rho_\downarrow}{\rho_\uparrow} \right) + \mathcal{O}(\rho^{\frac{7}{3}+\frac{1}{120}}) \ .$$

In order to prove Theorem 1, we need to estabilish a lower bound on $e(\rho_\uparrow, \rho_\downarrow)$ since the upper bound (2) has already been proved in [1]. The kinetic contribution and the first contribution to the leading order term are extracted by conjugation of the Hamiltonian $\mathcal{H}$ with the particle-hole transformation

$$R^* \widehat{a}_{k,\sigma} R = \begin{cases} \widehat{a}_{k,\sigma} \ , & \text{if } k \notin B_F^\sigma \\ \widehat{a}^*_{-k,\sigma} \ , & \text{if } k \in B_F^\sigma \end{cases}$$

on a normalized ground state Ψ of H_N such that $\mathcal{N}_\sigma \Psi = N_\sigma \Psi$. Thus, by first neglecting the equal spin contributions, we obtain

$$\langle \Psi, \mathcal{H}\Psi \rangle \geq E_{\mathrm{FFG}} + \langle R^*\Psi, \mathcal{H}_{\mathrm{corr}} R^*\Psi \rangle$$

where $\mathcal{H}_{\mathrm{corr}} = \mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_3 + \mathbb{Q}_4 + \mathcal{E}_{\mathrm{corr}}$ is the correlation hamiltonian with $\mathbb{Q}_j$ being quartic operators depending on the interaction V and

$$\lim_{L\to\infty} \frac{E_{\mathrm{FFG}}}{L^3} = \frac{3}{5}(6\pi^2)^{\frac{2}{3}} \left(\rho_\uparrow^{\frac{5}{3}} + \rho_\downarrow^{\frac{5}{3}} \right) + \hat{V}(0)\rho_\uparrow\rho_\downarrow + \mathcal{O}(\rho^{\frac{8}{3}})_{\rho\to 0} \ .$$

Moreover, the remainder $\mathcal{E}_{\mathrm{corr}}$ satisfies the bound $|\langle R^*\Psi, \mathcal{E}_{\mathrm{corr}} R^*\Psi \rangle| \leq C L^3 \rho^{\frac{7}{3}+\frac{1}{12}}$. The upper bound in [1] was proved by construction of a trial state, adapting the bosonic Bogoliubov theory to fermions and treating suitable pairs of fermions as (quasi-)bosonic excitations. The quasi-bosonic Bogoliubov transformation captures the ground state energy by approximately diagonalizing the Hamiltonian. The corresponding error terms are controlled by specific properties of the trial state. For the lower bound, the trial state method is not feasable since the available a-priori estimates for $\mathcal{N} = \sum_\sigma \sum_{k\in\mathbb{Z}^3} \widehat{a}^*_{k,\sigma}\widehat{a}_{k,\sigma}$ and $\mathbb{H}_0 = \sum_\sigma \sum_{k\in\mathbb{Z}^3} ||k|^2 - (k_F^\sigma)^2| \widehat{a}^*_{k,\sigma}\widehat{a}_{k,\sigma}$ on $R^*\Psi$ are insufficient to conclude a lower bound. The main obstruction to the application of the trial state method is given by the fact that the implementation of the Bogoliubov transformation produces several error terms of the form $\rho\mathcal{N}$ that can be bounded only by $\mathcal{O}(L^3\rho^{7/3})$ using the a-priori estimates. This is not sufficient to resolve the Huang-Yang conjecture. On the other hand, $\mathbb{Q}_3$ cannot be treated directly as an error term since a standard Cauchy-Schwarz estimate shows that the expectation value is bounded by $\mathcal{O}(L^3\rho^{7/3})$ while the corresponding expectation value on the trial state is zero. Instead, a completion of the square method is emploied. The Hamiltonian is decomposed into several terms in order to drop the non-negative ones of the form $|A|^2 := A^*A$ and obtain the lower bound. The first step in the completion of the square is the introduction of the corrections $T_\sigma(k)$ and $\mathcal{T}_{\sigma,\sigma'}(x,y)$ so that

(3)

$$\begin{aligned}\mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4 \approx & \sum_\sigma \sum_{k\in\mathbb{Z}^3} ||k|^2 - (k_F^\sigma)^2| |T_\sigma(k) + \widehat{a}_{k,\sigma}|^2 - \rho_\uparrow\rho_\downarrow L^3 \int_\Lambda V\varphi^2 - L^3 C_L(\rho_\uparrow, \rho_\downarrow) \\ & + \frac{1}{2}\sum_{\sigma\neq\sigma'} \int_{\Lambda^2} \mathrm{d}x\mathrm{d}y\, V(x-y) |a_{\sigma'}(u_y)a_\sigma(u_x) + \mathcal{T}_{\sigma,\sigma'}(x,y)|^2 + \mathcal{O}(\rho\mathcal{N})\end{aligned}$$

where $u_{\sigma,x}(\cdot) := u_\sigma(\cdot - x)$ is such that $\widehat{u}_\sigma(k) = \mathbb{1}_{(B_F^\sigma)^c}(k)$. The latter approximation is up to error terms controlled by the a-priori estimates. Moreover, the corrections are determined so that the constant $\hat{V}(0)\rho_\uparrow\rho_\downarrow$ in E_{FFG} combines with the constant $-\rho_\uparrow\rho_\downarrow \int_\Lambda V\varphi^2 - C_L(\rho_\uparrow, \rho_\downarrow)$ in (3) to give

$$(4)\quad \hat{V}(0)\rho_\uparrow\rho_\downarrow - \rho_\uparrow\rho_\downarrow \int_\Lambda V\varphi^2 - C_L(\rho_\uparrow, \rho_\downarrow) \geq 8\pi a\rho_\uparrow\rho_\downarrow + a^2\rho_\uparrow^{\frac{7}{3}} F\left(\frac{\rho_\downarrow}{\rho_\uparrow}\right) + \mathcal{O}(\rho^{\frac{7}{3}+\frac{1}{10}}).$$

The introduction of such corrections does not explain how to control $\mathbb{Q}_3$ and we still have the problem that $\mathcal{O}(\rho\mathcal{N})$ is bounded only by $\mathcal{O}(L^3\rho^{7/3})$ using the a-priori estimates. Therefore, it is necessary the introduction of other corrections $S_\sigma(k)$ and $\mathcal{S}_{\sigma,\sigma'}(x,y)$ such that $\mathbb{Q}_3$ is controlled, the $\mathcal{O}(\rho\mathcal{N})$ contributions from $|T_\sigma(k)|^2$ and $|\mathcal{T}_{\sigma,\sigma'}(x,y)|^2$ are cancelled out by the $\mathcal{O}(\rho\mathcal{N})$ contributions coming from $|S_\sigma(k)|^2$ and $|\mathcal{S}_{\sigma,\sigma'}(x,y)|^2$. The mixed terms involving $T_\sigma^*(k)S_\sigma(k)$ and $\mathcal{T}_{\sigma,\sigma'}^*(x,y)\mathcal{S}_{\sigma,\sigma'}(x,y)$ must be negligible. Thus, by means of the a-priori estimates, we consider

$$\begin{aligned}
\mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_3 + \mathbb{Q}_4 \approx &\sum_\sigma \sum_{k\in\mathbb{Z}^3} ||k|^2 - (k_F^\sigma)^2||T_\sigma(k) + S_\sigma(k) + \widehat{a}_{k,\sigma}|^2 \\
&+ \frac{1}{2}\sum_{\sigma\neq\sigma'} \int_{\Lambda^2} \mathrm{d}x\mathrm{d}y\, V(x-y)|a_{\sigma'}(u_y)a_\sigma(u_x) + \mathcal{T}_{\sigma,\sigma'}(x,y) + \mathcal{S}_{\sigma,\sigma'}(x,y)|^2 \\
&- \rho_\uparrow\rho_\downarrow L^3 \int_\Lambda V\varphi^2 - L^3 C_L(\rho_\uparrow, \rho_\downarrow)
\end{aligned}$$

which combined with the free Fermi gas energy E_{FFG}, dropping the non-negative terms and using (4) leads us to the proof of the lower bound for the ground state energy density. An open question would be to go beyond the second order correction in a, analyzing rigorously the next order corrections in a for the energy density.

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Thomas–Fermi theory and the limit of a large atom

Asbjørn Bækgaard Lauritsen

We introduce the Thomas–Fermi density theory for the energy of an atom and review the result of (Lieb and Simon, Adv. Math. 23.1 (1977); Lieb, Rev. Mod. Phys. 53.4 (1981)) that in the limit of large atomic number, the ground state energy of the neutral atom agrees with that predicted by Thomas–Fermi theory.

The atomic Hamiltonian. The Hamiltonian describing a system of N electrons in an external potential $-V$ is (with units where $\hbar = 1$ and $m = 1$)

$$H_N = \sum_{j=1}^{N} \left(-\frac{1}{2}\Delta_{x_j} - V(x_j) \right) + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|}$$

on the Hilbert space $\bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^q)$, where $q = 2$ is the number of spin-sectors. We shall mostly here be interested in the case of a neutral atom, where $V(x) = \frac{Z}{|x|}$ and $N = Z$. For such a system, a natural first question to ask is the evaluation of the ground state energy. We denote it by

$$E_Z = \inf_{\substack{\psi \in \bigwedge^N L^2(\mathbb{R}^3;\mathbb{C}^q) \\ \|\psi\|=1}} \langle \psi | H_Z \psi \rangle \,.$$

The Thomas–Fermi functional. Evaluating E_Z is in general a too complicated problem. One idea of approximating it is that given by Thomas and Fermi [1, 2]. Here one replaces $\langle \psi | H_Z \psi \rangle$ by a function of $\rho = \rho_\psi$, the one-particle density instead. To motivate the functional, we first write

$$\langle \psi | H_Z \psi \rangle = \operatorname{Tr}\left[-\frac{1}{2}\Delta \gamma_\psi^{(1)} \right] - \int V(x)\rho_\psi(x)\,\mathrm{d}x + \frac{1}{2}\iint \frac{1}{|x-y|}\rho_\psi^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y.$$

The second term is already of the desired form. For the last term, we simply approximate $\rho^{(2)}$ by the direct (i.e. Hartree) term: $\rho^{(2)}(x,y) \approx \rho(x)\rho(y)$. For the first term, we replace it by the semi-classical approximation

$$\operatorname{Tr}\left[-\frac{1}{2}\Delta\gamma^{(1)} \right] \approx \min_W \iint \frac{\mathrm{d}p\,\mathrm{d}x}{(2\pi)^3}\frac{p^2}{2}W(p,x) = \frac{3}{5}C^{\mathrm{TF}} \int \rho_\psi(x)^{5/3}\,\mathrm{d}x,$$

where W is minimized under the constraint $\int \frac{\mathrm{d}p}{(2\pi)^3} W(p,x) = \rho_\psi(x)$ and $W(p,x) \le q$, and $C^{\mathrm{TF}} = \frac{1}{2}\left(\frac{6\pi^2}{q}\right)^{2/3}$. This is easily solved ($W(\cdot, x)$ is a filled Fermi ball) giving the stated result. We arrive at

Definition 1. The *Thomas–Fermi functional* is

$$\mathcal{E}_Z^{\mathrm{TF}}(\rho) = \frac{3}{5}C^{\mathrm{TF}} \int \rho^{5/3}\,\mathrm{d}x - \int \frac{Z}{|x|}\rho(x)\,\mathrm{d}x + D(\rho,\rho),$$

where $D(\rho,\rho) = \frac{1}{2}\iint \frac{\rho(x)\rho(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y$. $\mathcal{E}^{\mathrm{TF}}$ is defined on the set $\{\rho \in L^1 \cap L^{5/3} : \rho \ge 0\}$.

Remark 2. The functional $\mathcal{E}_Z^{\mathrm{TF}}$ is convex and radial. Thus, a minimizer, if it exists, is unique and radial. Further, for any function $\rho_1(x)$ letting $\rho_Z(x) = Z^2\rho(Z^{1/3}x)$, we have the perfect scaling $\mathcal{E}_Z^{\mathrm{TF}}(\rho_Z) = Z^{7/3}\mathcal{E}_1^{\mathrm{TF}}(\rho_1)$. From the last point, it in particular follows that $E_Z^{\mathrm{TF}} := \inf_\rho \mathcal{E}_Z^{\mathrm{TF}}(\rho) = Z^{7/3}E_1^{\mathrm{TF}}$.

Lemma 3 ([3, Section II])**.** *There exists a unique minimizer ρ^{TF} of the Thomas–Fermi functional $\mathcal{E}_Z^{\mathrm{TF}}$. It satisfies*

$$\int \rho^{\mathrm{TF}}\,\mathrm{d}x = Z, \qquad C^{\mathrm{TF}}\rho^{2/3} = \phi^{\mathrm{TF}} := V - \rho^{\mathrm{TF}} * \frac{1}{|x|},$$

where $*$ denotes the convolution and ϕ^{TF} is called the Thomas–Fermi potential.

The limit of a large atom. We consider next the energy E_Z in the limit of large atomic number (and number of electrons) $Z \to \infty$. Here one has

Theorem 4. *In the limit $Z \to \infty$ we have*

$$E_Z = E_Z^{\mathrm{TF}} + o(Z^{7/3}) = Z^{7/3}E_1^{\mathrm{TF}} + o(Z^{7/3}).$$

This result is due to Lieb and Simon [5]. We give here a sketch of proof following [3].

Sketch of proof —— upper bound. Note first that, since Slater determinants are quasi-free,

$$E_Z = \inf_{\psi} \langle \psi | H_Z \psi \rangle \le \inf_{\psi \text{ Slater}} \langle \psi | H_Z \psi \rangle = \inf_{\substack{\gamma \text{ projection} \\ \mathrm{Tr}\,\gamma = Z}} \mathcal{E}^{\mathrm{HF}}(\gamma),$$

where

$$\mathcal{E}^{\mathrm{HF}}(\gamma) = \mathrm{Tr}\left[-\frac{1}{2}\Delta\gamma\right] - \int V\rho_\gamma + \frac{1}{2}\iint \frac{\rho_\gamma(x)\rho_\gamma(y) - \sum_{\sigma,\tau}|\gamma(x,\sigma;y,\tau)|^2}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y$$

is the Hartree–Fock functional. Next, we use

Lemma 5 (Lieb variational principle [4])**.**

$$\inf_{\substack{\gamma \text{ projection} \\ \mathrm{Tr}\,\gamma = Z}} \mathcal{E}^{\mathrm{HF}}(\gamma) = \inf_{\substack{0 \le \gamma \le 1 \\ \mathrm{Tr}\,\gamma = Z}} \mathcal{E}^{\mathrm{HF}}(\gamma).$$

Lastly, the exchange term (with $\ldots |\gamma|^2$) is negative, so we may drop it for an upper bound. To construct a trial state we use coherent states. Hence, let g be a radial, compactly supported function with $\int |g|^2 = 1$ (think $|g|^2$ an approximate δ-function) and consider the coherent states $f_{pr}(x) = g(x-r)e^{ipx}$. We choose as a trial state (for some function ρ to be chosen)

$$\gamma = \iint \frac{\mathrm{d}p\,\mathrm{d}r}{(2\pi)^3}\chi\left(\frac{p^2}{2} - C^{\mathrm{TF}}\rho(r)^{2/3} \le 0\right)|f_{pr}\rangle\langle f_{pr}| \otimes \mathbb{1}_{\mathrm{spin}}.$$

One easily verifies that this is a valid trial state. Moreover,

$$\rho_\gamma(x) = \rho * |g|^2, \qquad \mathrm{Tr}\left[-\frac{1}{2}\Delta\gamma\right] = \frac{3}{5}C^{\mathrm{TF}}\int \rho^{5/3} + \frac{1}{2}Z\int |\nabla g|^2.$$

Next, $|g|^2 * \frac{1}{|x|} * |g|^2 \le \frac{1}{|x|}$ as a convolution operator by Fourier transforming. Hence,

$$D(\rho_\gamma, \rho_\gamma) = \frac{1}{2}\int \rho_\gamma * \frac{1}{|x|} * \rho_\gamma = \frac{1}{2}\int \rho * |g|^2 * \frac{1}{|x|} * |g|^2 * \rho \le D(\rho,\rho).$$

Combining the above ideas, we find

$$E_Z \le \mathcal{E}_Z^{\mathrm{TF}}(\rho) + \frac{Z}{2}\int |\nabla g|^2 + \int (V - V * |g|^2)\rho.$$

Choosing $\rho = \rho^{\mathrm{TF}}$ and optimizing in the choice of g proves the upper bound in Theorem 4.

Sketch of proof —— lower bound. First, we have

Lemma 6 (Lieb–Oxford inequality [6, 7]). *For some $C_{\mathrm{LO}} > 0$ we have for all ψ*

$$\left\langle \psi \middle| \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|}\psi \right\rangle \ge D(\rho_\psi, \rho_\psi) - C_{\mathrm{LO}} \int \rho_\psi^{4/3}\,\mathrm{d}x.$$

Next, since $D(\cdot,\cdot)$ is a positive quadratic form (by Fourier transforms), we have for any $\tilde\rho$

$$0 \le D(\rho_\psi - \tilde\rho, \rho_\psi - \tilde\rho) = D(\rho_\psi, \rho_\psi) + D(\tilde\rho, \tilde\rho) - \int \tilde\rho * \frac{1}{|x|}\rho_\psi.$$

Combining the above ideas we find, with effective potential $\tilde\phi = V - \tilde\rho * \frac{1}{|x|}$, for any ψ

$$\langle \psi | H_Z \psi\rangle \ge \operatorname{Tr}\left((1-\epsilon)\frac{-\Delta}{2} - \tilde\phi\right)\gamma_\psi^{(1)} - D(\tilde\rho,\tilde\rho) + \epsilon \operatorname{Tr}\left[\frac{-\Delta}{2}\gamma_\psi^{(1)}\right] - C_{\mathrm{LO}}\int \rho_\psi^{4/3}.$$

Here we borrowed ϵ of the kinetic energy in order to bound some appearing error terms. To bound the first term, we use again coherent states. Letting again g be a radially compactly supported function with $\int |g|^2 = 1$ and $f_{pr}(x) = g(x-r)e^{ipx}$ we have for any m with $\int |m|^2 = 1$

$$\begin{aligned}\int \frac{1}{2}|\nabla m|^2 &= \iint \frac{p^2}{2}\langle m|f_{pr}\rangle\langle f_{pr}|m\rangle \frac{\mathrm{d}p\,\mathrm{d}r}{(2\pi)^3} - \frac{1}{2}\int |\nabla g|^2,\\ \int |m|^2 F * |g|^2 &= \iint F(r)\langle m|f_{pr}\rangle\langle f_{pr}|m\rangle \frac{\mathrm{d}p\,\mathrm{d}r}{(2\pi)^3}.\end{aligned}$$

Let $e_1(\psi) = e_1(M_\psi) - \frac{Z}{2}\int |\nabla g|^2$ denote the first term above, where $\tilde\phi$ has been replaced by $\tilde\phi * |g|^2$, and where $M_\psi(p,r) = \operatorname{Tr}\gamma_\psi^{(1)}|f_{pr}\rangle\langle f_{pr}|$. We note that M_ψ satisfies $\iint \frac{\mathrm{d}r\,\mathrm{d}p}{(2\pi)^3}M = Z$ and $M(r,p) \le q$. Taking these conditions as constraints for a semi-classical density M, we have

$$\inf_\psi e_1(\psi) - D(\tilde\rho,\tilde\rho) \ge \inf_M e_1(M) - D(\tilde\rho,\tilde\rho) - \frac{Z}{2}\int |\nabla g|^2 = \tilde{\mathcal{E}}_Z^{\mathrm{TF}}(\tilde\rho) - \frac{Z}{2}\int |\nabla g|^2,$$

by simple calculations, if $\tilde\rho$ is taken as the Thomas–Fermi density for the problem where C^{TF} is replaced by $(1-\epsilon)C^{\mathrm{TF}}$, and $\tilde{\mathcal{E}}_Z^{\mathrm{TF}}$ denotes the functional with the same replacement. Up to the factor ϵ this term gives the desired lower bound.

Finally, to bound all the errors, we use the saved ϵ of kinetic energy and the Lieb–Thirring inequality [8]. After optimizing in the choice of g and ϵ we conclude the lower bound in Theorem 4.

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Ground state energy of a charged Fermi gas at high density

Francois Visconti

In this talk, we consider a system of N fermions trapped in a box $\Lambda \subset \mathbb{R}^3$ in the presence of a uniform charge background with total charge N. The system is described by the action of the Hamiltonian

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

on $L^2_{\mathrm{a}}(\Lambda^N)$, the N-fold antisymmetric tensor product of $L^2(\Lambda)$. A wavefunction $\Psi \in L^2(\Lambda^N)$ is in $L^2_{\mathrm{a}}(\Lambda)$ if and only if it satisfies

$$\Psi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = -\Psi(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_N),$$

for any pair of indices (i, j). The operator $-\Delta$ is the Laplacian with Dirichlet boundary conditions on Λ, and the potential V is taken of the form

$$V(x) = \frac{N}{|\Lambda|} \int_{\Lambda} \frac{\mathrm{d}y}{|x - y|}.$$

This potential describes the interactions of the electrons, which are taken to have charge -1, with a uniform background that has total charge N. This is called a neutral jellium model.

The ground state energy $E_N(\Lambda)$ of H_N is defined by

$$E_N(\Lambda) = \inf \left\{ \langle \Psi, H_N \Psi \rangle : \Psi \in L^2_{\mathrm{a}}(\Lambda^N), \|\Psi\| = 1 \right\}.$$

We study the thermodynamic ground state energy per unit volume of the system with the self-energy of the background included:

$$e_{\mathrm{J}}(\overline{\rho}) = \lim_{\substack{N,|\Lambda|\to\infty \\ N/|\Lambda|=\overline{\rho}}} |\Lambda|^{-1}\left(E_N(\Lambda) + \frac{1}{2}\iint_{\Lambda^2} \mathrm{d}x\mathrm{d}y \frac{\overline{\rho}^2}{|x-y|}\right). \tag{1}$$

That this limit exists and is independent of the shape of Λ was proven in [7]. We are interested in the high-density regime $\overline{\rho}\to\infty$. The main result presented in the talk is the following from [6].

Theorem 1. *Let $\overline{\rho} \geq C$. Then*

$$e_{\mathrm{J}}(\overline{\rho}) = \frac{3}{5}c_{\mathrm{TF}}\overline{\rho}^{5/3} - c_{\mathrm{D}}\overline{\rho}^{4/3} - C(\overline{\rho})\rho^{4/3}, \tag{2}$$

with $c_{\mathrm{TF}} = (6\pi^2)^{2/3}, c_{\mathrm{D}} = (2\pi)^{-3}c_{\mathrm{TF}}^2$ and $0 \leq C(\overline{\rho}) \leq C_\varepsilon \overline{\rho}^{-1/15+\varepsilon}$, for any $\varepsilon > 0$ small enough.

The first term in the expansion (2) is called the Thomas–Fermi term, and the second is called the Dirac term [4]. To see where this expansion comes from, we use Hartree–Fock theory. Namely, we restrict our attention to Slater determinants, or said differently to wavefunctions of the form

$$\Psi = u_1 \wedge \cdots \wedge u_N,$$

for some orthonormal family $u_1,\ldots,u_N$. The 1-particle reduced density matrix of Ψ is the projection P on the N-dimensional space spanned by $(u_1,\ldots,u_N)$, and the corresponding 1-body density is $\rho_P(x) = P(x;x)$, where $P(x;y)$ denotes the integral kernel of P. Moreover, the 2-body density of Ψ can also be computed explicitly and is given by

$$\rho^{(2)}(x,y) = \frac{1}{2}\rho_P(x)\rho_P(y) - \frac{1}{2}|P(x;y)|^2. \tag{3}$$

Thus, the expectation $\langle\Psi, H_N\Psi\rangle$ is equal to the Hartree Fock energy

$$\mathcal{E}^{\mathrm{HF}}[P] = \mathrm{Tr}((-\Delta - V)P) + D(\rho_P,\rho_P) - \frac{1}{2}\iint_{\Lambda^2} dx\,\mathrm{d}y \frac{|P(x;y)|^2}{|x-y|},$$

where we introduced the quadratic form

$$D(\rho_1,\rho_2) = \frac{1}{2}\iint_{\Lambda^2} \mathrm{d}x\,\mathrm{d}y \frac{\rho_1(x)\rho_2(y)}{|x-y|}.$$

The term involving the quadratic form D is called the direct energy, and the last term is called the exchange energy. Adding the self-energy of the background, we find

$$\mathcal{E}^{\mathrm{HF}}[P] + D(\overline{\rho},\overline{\rho}) = \mathrm{Tr}(-\Delta P) + D(\rho_P - \overline{\rho}, \rho_P - \overline{\rho}) - \frac{1}{2}\iint_{\Lambda^2} \mathrm{d}x\,\mathrm{d}y \frac{|P(x;y)|^2}{|x-y|}. \tag{4}$$

To obtain (2) we use as a trial state a Slater determinant of the N lowest eigenvalues of $-\Delta$ on Λ, which is often referred to as filling the Fermi ball (see Figure 1). The density of such a trial state approaches the uniform density $\overline{\rho}$ in the thermodynamic limit, and thus the term $D(\rho_P - \overline{\rho}, \rho_P - \overline{\rho})$ vanishes. Moreover, in the same limit, the radius of the Fermi ball, called the Fermi radius k_F, converges to $c_{\mathrm{TF}}\overline{\rho}^{1/3}$, and the gap between the points of the lattice goes to zero. Hence, computing the kinetic energy of our trial state amounts to integrating the momentum squared over a ball of radius $c_{\mathrm{TF}}\overline{\rho}^{1/3}$, which precisely gives the first term in (2). Though computing the second term in the expansion is more tedious, we can still explain heuristically why it is of order $\overline{\rho}^{4/3}$. When putting $\rho^{(2)}$ into the form (3), we added and removed the self-energy of the electrons to reconstruct the direct term $\frac{1}{2}\rho_P(x)\rho_P(y)$. This means that, amongst other things, the exchange term $|P(x;y)|^2$ contains this self-energy. Since each of these electrons lives on a length scale $\overline{\rho}^{-1/3}$, the self-energy of a single electron is expected to be of order $\overline{\rho}^{1/3}$. Multiplying this by the density $\overline{\rho}$ of electrons, we get a contribution of order $\overline{\rho}^{4/3}$.

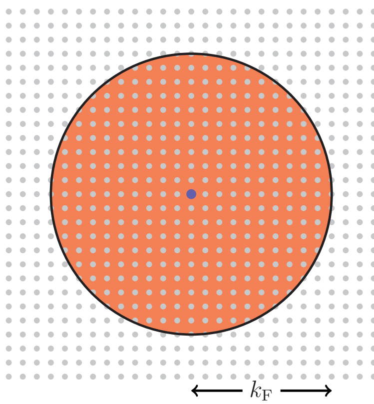

FIGURE 1. Illustration of the Fermi ball for $\Lambda = [0, L]^3$ with periodic boundary conditions. The eigenvalues of $-\Delta$ are exactly given by p^2, for all points p in the lattice $(2\pi\mathbb{Z}/L)^3 \setminus \{0\}$. (represented in grey). The Fermi ball (red) is obtained by taking the N points closest to the origin (blue), which defines the Fermi radius k_{F}. In the thermodynamic limit, the gap between the lattice points closes, so the variable p becomes continuous in a ball of radius $c_{\mathrm{TF}}\overline{\rho}^{1/3}$.

Though the heuristics described above can be made rigorous and in particular imply the nonnegativity of $C(\rho)$ in (2), they only give an upper on the ground state energy. Proving a matching lower bound is a much more difficult task, and the key ingredient from [6] is a correlation estimate that states

$$\left\langle \Psi, \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|}\Psi \right\rangle \ge D(\rho^{(1)}, \rho^{(1)}) - \frac{1}{2}\iint_{\Lambda^2} \mathrm{d}x\,\mathrm{d}y \frac{|P(x;y)|^2}{|x-y|} - \text{error}, \tag{5}$$

for any normalised $\Psi \in L^2_{\rm a}(\Lambda^N)$ with 1-body density $\rho^{(1)}$, and any density matrix P that satisfies $0 \leq P \leq \mathbb{1}$ and $\operatorname{Tr} P < \infty$. Taking Ψ to be an approximate ground state of H_N and P to be the same projection on the Fermi ball as before, and controlling the errors, we obtained the desired lower bound.

The correlation estimate (5) follows from a more general algebraic inequality, which is the key novelty of [6]. This inequality is actually a generalisation of an estimate by Bach [1], which was used to prove the validity of Hartree–Fock theory for molecules in the Born–Oppenheimer approximation at high density.

Finally, a perturbative computation of Gell–Mann and Brueckner [5] suggests that the third and fourth order corrections in (2) should be given by

$$c_1\overline{\rho}\log\overline{\rho} + c_2\overline{\rho} + o(\overline{\rho}),$$

for some specific constants c_1 and c_2. Recently, this formula was established rigorously in [2, 3] for systems in the mean-field regime, i.e. described by a Hamiltonian acting on the unit torus and with a prefactor $k_{\rm F}^{-1}$ in front of the interaction potential. Though the analysis of the lower bound even goes slightly beyond the mean-field regime, covering prefactors of the form $k_{\rm F}^{-1+\varepsilon}$ for $\varepsilon > 0$ small, it remains an open problem to establish the Gell–Mann–Brueckner formula in the thermodynamic limit.

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Correlation energy of an electron gas in the mean-field approximation

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The correlation energy of a high density fermionic Coulomb gas, called Jellium, in the thermodynamic limit is expected to be given by the Gell-Mann–Brueckner formula [6].

$$E_{corr} = E_N - E_{HF} = c_1\rho\log\rho + c_2\rho\ ,$$

for explicit constants c_1, c_2. While a rigorous derivation of such a formula from first principles remains an open problem in mathematical physics, in the lecture we focus on a rigorous upper bound for the correlation energy of a mean-field Fermi gas with bounded interaction, following the bosonization method developed in [3].

1. Setting and Statement of the Main Result

We consider a system of N spinless fermions on the torus $\mathbb{T}^3 = [0, 2\pi]^3$ (with periodic boundary conditions) interacting via a pairwise potential $V : \mathbb{T}^3 \to \mathbb{R}$ with Fourier coefficients satisfying

$$\forall k \in \mathbb{Z}^3_* : \quad \hat{V}_k \geq 0\,, \quad \hat{V}_k = \hat{V}_{-k}\,, \quad \sum_{k \in \mathbb{Z}^3_*} |k| \hat{V}_k < +\infty\,. \tag{1}$$

We also assume that $\hat{V}_0 = 0$, or equivalently the "background" has been subtracted. The system is described by the Hamiltonian

$$H_N := H_{kin} + k_F^{-1} H_{int} = \sum_{i=1}^{N} (-\Delta_i) + k_F^{-1} \sum_{1 \leq i < j \leq N} V(x_i - x_j) \tag{2}$$

acting on the fermionic Hilbert space $\mathcal{H}_N = \bigwedge^N L^2(\mathbb{T}^3)$.

Here the coupling constant k_F^{-1} corresponds to the interaction strength, and the mean-field regime arises when the kinetic and interaction energies are comparable, i.e. $k_F^{-1} \sim N^{-1/3}$. More precisely, we assume the Fermi ball B_F to be completely filled by N integer points:

$$B_F = \mathbb{Z}^3 \cap \overline{B(0, k_F)}\,, \quad N = |B_F| = \frac{4\pi}{3} k_F^3 (1 + o(1)_{k_F \to \infty})\,. \tag{3}$$

We study the ground state energy $E_N := \inf \sigma(H_N)$ in the limit $k_F \to \infty$.

In this case, the kinetic operator H_{kin} has a unique, non-degenerate ground state given by the Fermi state

$$\psi_{FS} = \bigwedge_{p \in B_F} u_p\,, \quad u_p(x) = (2\pi)^{-3/2} e^{ip \cdot x}\,. \tag{4}$$

In this scaling, ψ_{FS} is also the Hartree–Fock minimizer (see Appendix A of [1]). Thus, to obtain the correction to the energy of the Fermi state we need to understand the correlation structure of the system. In the lecture we sketch the proof of the following (part of Theorem 1.1 in [3]):

Theorem. Define for each $k \in \mathbb{Z}^3_*$ the *lune*

$$L_k := \left\{ p \in \mathbb{Z}^3 \mid |p - k| \leq k_F < |p| \right\} = (B_F + k) \setminus B_F\,, \quad \lambda_{k,p} := \frac{1}{2}(|p|^2 - |p - k|^2)\,.$$

In the setting above: as $k_F \to \infty$, it holds that

$$E_N \leq E_{FS} + E^{Bos}_{corr} + o(k_F)\,, \tag{5}$$

where the bosonic contribution to the correlation energy is defined by

$$E^{Bos}_{corr} = \frac{1}{\pi} \sum_{k \in \mathbb{Z}^3_*} \int_0^\infty F\left(\frac{\hat{V}_k k_F^{-1}}{(2\pi)^3} \sum_{p \in L_k} \frac{\lambda_{k,p}}{\lambda_{k,p}^2 + t^2} \right) dt\,, \quad F(x) = \log(1 + x) - x\,. \tag{6}$$

Remarks

(1) The Fermi energy E_{FS} contains the kinetic energy of order k_F^5 and the exchange interaction of order k_F^2. By Taylor expanding $F(x) \approx -x^2/2$ one can see that, under our regularity assumption (1), $E_{corr}^{Bos} \sim k_F$.
(2) If we formally perform in E_{corr}^{Bos} the substitutions $k_F^{-1}\hat{V}_k \to 4\pi e^2|k|^{-2}$ and $(2\pi)^3 \to$ the volume of the box and we take the thermodynamic limit, we get the first term of the Gell-Mann–Brueckner formula $c_1\rho\log(\rho)$.
(3) The authors of [3] also prove the matching lower bound. The approach was later extended in [4] to deal with more singular potentials $\hat{V}_k \in \ell^2(\mathbb{Z}_*^3)$ (including Coulomb), recovering the equivalent of the second term $c_2\rho$ as un upper bound. The matching lower bound has been obtained in [5] with a different method.
(4) The same result as above, together with the matching lower bound, has been obtained with a different bosonization method in [2].

2. Overview of the proof

Rewriting the Hamiltonian. Using the second quantization formalism, we can normal order H_N in (2) with respect to ψ_{FS}. More precisely, we obtain

$$H_N = E_{FS} + H'_{kin} + \frac{k_F^{-1}}{2(2\pi)^3}\sum_{k\in\mathbb{Z}_+^3}\hat{V}_k\left(2B_k^*B_k + B_kB_{-k} + B_{-k}^*B_k^*\right) + H_{NB}\ , \tag{7}$$

where we have defined the localized kinetic energy

$$H'_{kin} := H_{kin} - \langle\psi_{FS}, H_{kin}\psi_{FS}\rangle = \sum_{p\notin B_F}|p|^2a_p^*a_p - \sum_{p\in B_F}|p|^2a_pa_p^*\ , \tag{8}$$

and the quasi-bosonic averaged operator

$$B_k := \sum_{p\in L_k} b_{k,p}\ , \qquad b_{k,p} := a_{p-k}^*a_p \quad \forall p\in L_k\ . \tag{9}$$

These satisfy approximate Canonical Commutation Relations (CCR) in an average sense, namely

$$|L_k|^{-1}[B_k, B_l^*] = \delta_{k,l} - \frac{1}{|L_k|}\left(\sum_{p\in L_k\cap L_l} a_{p-l}a_{p-l}^* + \sum_{p\in L_k\cap(L_l-l+k)} a_{p-k+l}^*a_p\right)\ ,$$

and the second term in the right-hand side is much smaller than one in expectation value on approximate ground states, see section 1.2 of [3].
The term H_{NB} falls outside the quasi-bosonic picture and is therefore considered an error term to be analyzed separately at the end.
To include H'_{kin} in the quasi-bosonic picture, we observe that for each $p\in L_k$

$$\left[H'_{kin}, b_{k,p}^*\right] = 2\lambda_{k,p}b_{k,p}^*\ , \quad \Longrightarrow \quad H'_{kin} \sim 2\sum_{k\in\mathbb{Z}_*^3}\sum_{p\in L_k}\lambda_{k,p}b_{k,p}^*b_{k,p}\ . \tag{10}$$

Diagonalizing the bosonizable terms. In analogy with the bosonic case, we find that for the right choice of symmetric operators $K_l : \ell^2(L_l) \to \ell^2(L_l)$, the kernel

$$\mathcal{K} = \frac{1}{2} \sum_{l \in \mathbb{Z}^3_*} \sum_{p,q \in L_l} \langle e_p, K_l e_q \rangle \left(b_{l,p} b_{-l,-q} - b^*_{-l,-q} b^*_{l,p} \right) \ ,$$

satisfies the diagonalization condition

$$e^{\mathcal{K}} \left(H'_{kin} + \frac{k_F^{-1}}{2(2\pi)^3} \sum_{k \in \mathbb{Z}^3_*} \hat{V}_k \left(2B^*_k B_k + B_k B_{-k} + B^*_{-k} B^*_k \right) \right) e^{-\mathcal{K}} =$$
$$= E^{Bos}_{corr} + H'_{kin} + \sum_{k \in \mathbb{Z}^3_*} \sum_{p,q \in L_k} \langle e_p, E_k e_q \rangle b^*_{k,p} b_{k,q} + \mathcal{E}_{exch.} \ .$$

Here the exchange error $\mathcal{E}_{exch.}$ arises precisely from the fact that the operators $b_{k,p}$ do not satisfy exact Canonical Commutation Relations.

Bounding the error terms. . We want to take as a trial state $e^{-\mathcal{K}} \psi_{FS}$: using that $H'_{kin} \psi_{FS} = 0 = b_{k,p} \psi_{FS}$, the final step is to show

$$\langle \psi_{FS}, e^{\mathcal{K}} H_{NB} e^{-\mathcal{K}} \psi_{FS} \rangle \, , \, \langle \psi_{FS}, \mathcal{E}_{exch.} \psi_{FS} \rangle \leq o(k_F) \ . \tag{11}$$

These bounds constitute one of the main technical difficulties in [3].

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