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BOSE–EINSTEIN CONDENSATION: A TRANSITION TO CHAOS RESULT

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Abstract. Within a stochastic approach to Bose-Einstein Condensation we point out some probabilistic counterparts of the relevant analytical results due to Lieb, Yngvason and Seiringer about the behaviour of the quantum N-body ground state energy under the so called Gross-Pitaevskii scaling limit. In particular we focus our attention on a transition to chaos result for the rigorously associated interacting N-particles system.

1. Introduction

The first experimental realization of the long-predicted Bose-Einstein condensation (BEC) was obtained in 1995. This quantum phenomenon, in fact, has been discovered 70 years before within the mathematical background of Quantum Mechanics. The basic idea was certainly due to Bose ([7]) in 1924, who proposed a new quantum statistical description of photons as indistinguishable particles. In 1925 Einstein ([16]), on the base of Bose's work, made the first proper prediction of the strange phenomenon for a gas of non-interacting atoms and, successively, also for massive particles.

In recent experiment ([27],[12]) a large amount of interacting Bose particles of certain chemical species are confined in a trap at a suitable high dilution. When the temperature is sufficiently low, the particles begin to behave *as if* almost all of them were in the same quantum state, called the condensate state.

Some semi-rigorous mathematical treatment of the problem was due to Bogoliubov ([6]) and others during the 1950s and 1960. In particular Gross and Pitaevskii in 1960 ([24],[41]) successfully proposed to model the many-body effects in the condensate regime by a non linear on-site self interaction between particles depending on the particle density itself. This gives rise to a peculiar non linear Schrödinger equation obeyed by the condensate wave function.

On the mathematically rigorous level, the Gross-Pitaevskii (GP) theory has been verified only for the *ground state* of the trapped interacting Bose gas by Lieb, Seiringer and Yngvason (2001,[29]) and by Lieb, Seiringer (2002,[30]), within

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the standard Quantum Mechanics. This important physical mathematical result succeeded in proving BEC from first principles, at least for the ground state, by performing an appropriate scaling limit of infinite particles starting from the original many-body Hamiltonian. See finally [1], [18] and [28] for the approach to the time-stability of condensation and, in particular, for the derivation of the time-dependent Gross-Pitaevskii equation. In [35] one can find a complete review of the analytical mathematical aspect of BEC.

As regards the stochastic approaches to BEC, the main research's line is that of random point processes, Boson fields or general Cox processes either in the ideal case ([22],[21],[20],[46],[17],[47],[49]), or in the interacting case ([48]) and also within a Statistical Mechanics framework ([23]).

More recently other interesting descriptions were proposed. In [4], the authors exploit models of spatial random permutations in relation to Feyman-Kac representation of the quantum Bose gas. In [2] a model of N mutually repellent Brownian Motions confined in a bounded space region is studied by a large deviation principle.

Very recently BEC has been studied within Nelson's Stochastic Mechanics in the usual three-dimensional space. In [37] the interacting N-particles systems, which can be rigorously associated to the quantum N-body Hamiltonian, was analyzed in connection with the GP scaling limit. Precisely, starting from the N-body quantum Hamiltonian, one can show that under the assumption of strictly positivity and continuous differentiability of the many-body ground state wave function, it is possible to rigorously defined an one-particle stochastic process, unique in law, which describes the motion of a single particle in the condensate gas. In the GP scaling limit, the one-particle process continuously remains outside a time dependent random *interaction set* with probability one and its stopped version converges, in a relative entropy sense, toward a Markov diffusion whose drift is uniquely determined by wave function of the condensate.

In this paper we focus our attention on a transition to chaos result which says that the sequence of symmetric probability measures describing our interacting N-particles system is *chaotic* with respect to the limit probability measure uniquely associated to the condensate wave function. The same probabilistic notion can be expressed by proving a sort of law of large numbers satisfied by the (random) *empirical measures* of the N particles, which provides their spatial empirical distribution, when the particles number goes to infinity.

The paper is organized as follows.

In Section 2 we briefly recall the Nelson stochastic approach to quantum mechanical treatment of the general N-body problem and we introduce the uniquely associated interacting N-particles system. We also describe the Gross-Pitaevskii quantum description of the BEC regime.

In Section 3 we explain the so called GP scaling limit and recall some fundamental analytical results due to Lieb, Yngvason and Seiringer regarding the behaviour of the N-particles mean ground-state energy under this limit: the *Energy Theorem*, the *Energy Localization Theorem* and the *BEC Theorem*. While the first affirms the convergence of the mean ground state energy to the GP energy, the second states that, asymptotically, the *finite* kinetic energy of a single particle, and precisely the part due to interaction, is concentrated on small balls centered on the points where the other particles are localized. Finally the *BCE Theorem* proves that the n-reduced density matrix factorizes in the scaling limit. In particular we report in Appendix the full proofs of the *Energy* and *Energy Localization Theorems*, because of the essential role the theorems play in the stochastic framework too.

In section 4 we show that the *BEC Theorem* allows to prove that our interacting particles system under the GP scaling limit performs a *transition to chaos* with respect to a natural asymptotic probability density. Moreover we recall the alternative suggestive formulation of the same result in terms of the *empirical measures* of our interacting diffusions.

In Section 5 we define the one-particle process, a three dimensional diffusion uniquely associated to the GP functional through the wave function of the condensate. Successively we introduce a suitable one particle relative entropy and describe its behaviour in the GP asymptotic scenario.

2. Nelson Map and Bose-Einstein Condensation

Nelson's Stochastic Mechanics allows to study quantum phenomena using diffusion processes instead of the standard analytical tools of Quantum Mechanics. While the formal stochastic equations have been firstly introduced by Fényes ([19]), Nelson ([40]) was able to introduce a complete stochastic mechanical theory representing nowadays an alternative approach to Quantum Mechanics. See [10] for a very recent review on Stochastic Mechanics.

We will briefly explain the *Nelson map* that associates a well-defined diffusion process to a solution of a Schrödinger equation.

Let $\psi(x,t)$ be a solution of the equation:

$$i\partial_t\psi(x,t) = H\psi(x,t) \tag{2.1}$$

with $\psi(x,0) = \psi_0(x)$, corresponding to the Hamiltonian operator:

$$H = -\frac{\hbar^2}{2m}\triangle + V(x), \tag{2.2}$$

where m denotes the mass of a particle, and V is some scalar potential.

Denoting by:

$$u(x,t) = Re[\frac{\nabla\psi(x,t)}{\psi(x,t)}] \tag{2.3}$$

$$v(x,t) = Im[\frac{\nabla\psi(x,t)}{\psi(x,t)}] \tag{2.4}$$

when $\psi(x,t) \neq 0$ and, otherwise, both $u(x,t)$ and $v(x,t)$ are set equal to zero. Let us put

$$b(x,t) := u(x,t) + v(x,t). \tag{2.5}$$

Let $(\Omega, \mathcal{F}, \mathcal{F}_t, X_t)$, with $\Omega = C(\mathbb{R}_+, \mathbb{R}^3)$, be the evaluation stochastic process $X_t(\omega) = \omega(t)$, with $\mathcal{F}_t = \sigma(X_s, s \leq t)$ the natural filtration.

Carlen ([9], Thm 2.1) proved that if the scalar potential V is a Rellich class potential and $\|\nabla\psi_0\|^2 < +\infty$, then there exists a unique Borel probability measure $\mathbb{P}$ on Ω such that

i)$(\Omega, \mathcal{F}, \mathcal{F}_t, X_t, \mathbb{P})$ is a Markov process;

ii) the image of $\mathbb{P}$ under X_t has density $\rho(t,x) := |\psi(x,t)|^2$;

iii) $W_t := X_t - X_0 - \int_0^t b(X_s, s)ds$

is a $(\mathbb{P}, \mathcal{F}_t)$-Brownian Motion.

For a generalization to the case of Hamiltonian operators with magnetic potential see [42](Thm.2.2).

The continuity of the above *Nelson-Carlen map*, with respect to the total variation norm, when a sequence of scalar potentials $V_n(t)$ converges in the Rellich class, has been proved in [13]. For the extension to the electromagnetic case see [42].

It is well known that Stochastic Mechanics is a real Newtonian Mechanics. In fact Nelson ([40]), having introduced a natural mean stochastic acceleration a_N, proved that the diffusion X satisfies the stochastic version of the second Newton's law

$$a_N(X_t) = -\frac{1}{m}\nabla V(X_t). \tag{2.6}$$

Moreover Guerra and Morato showed that X is critical for the mean classical action functional ([26]). For the stochastic variational principles see also [36],[26], [33] and [38].

Finally we recall that the generator of the Nelson diffusion is related to the Hamiltonian H by a Doob's transformation ([14] and [44] (Ch.VIII,Prop.3.9)). See [3] for the explicit formulation of Doob's transformation in a general Stochastic Mechanics setting.

We adopt the following notations: capital letters for stochastic processes or, otherwise, we will explicitly specify them, $\hat{X} = (X_1, ..., X_N)$ to denote arrays in $\mathbb{R}^{3N}$ and bold letters for vectors in $\mathbb{R}^3$.

In order to correctively model the recent experiments ([27],[12]) on BEC we start from the following N-body Hamiltonian

$$H_N = \sum_{i=1}^{N}(-\frac{\hbar^2}{2m}\triangle_i + V(\mathbf{r_i})) + \sum_{1\le i<j\le N} v(\mathbf{r_i} - \mathbf{r_j}), \tag{2.7}$$

where V is a confining potential and v a pair-wise repulsive interaction potential. As it is suitable for Bose particles it operates on symmetric wave functions in $L^2(\mathbb{R}^{3N})$. Being the physical experiments realized at very low temperature, a ground state approach to (2.7) is physically justified.

We consider the mean quantum mechanical energy

$$E[\Psi] = T_\Psi + \Phi_\Psi, \tag{2.8}$$

where

$$T_\Psi = \sum_{i=1}^{N}\int_{\mathbb{R}^{3N}} |\nabla_i\Psi|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N \tag{2.9}$$

is physically called the *kinetic energy* and

$$\Phi_\Psi = \sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} V(\mathbf{r}_i)|\Psi|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N + \frac{1}{2}\sum_{i=2}^{N} \int v(\mathbf{r}_1 - \mathbf{r}_i)|\Psi|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N \quad (2.10)$$

the *potential energy*. The variational problem associated to H_N consists in minimizing $E[\Psi]$ with respect to the complex-valued function Ψ in $L^2(\mathbb{R}^{3N})$ subject to the constrain $\|\Psi\|_2 = 1$. If such a minimizing function Ψ_N^0 exists it is called a *ground state*. The corresponding energy $E_0[\Psi_N^0]$ given by

$$E_0[\Psi_N^0] := \inf\{E(\Psi) : \int |\Psi|^2 = 1\} \quad (2.11)$$

is known as *ground state energy*.

Under suitable assumptions on the potentials V and v one can prove the existence of the ground state Ψ_N^0 of (2.7). As concerns uniqueness of the ground state we mean that it is unique apart from an *overall phase*. For our purpose we need a strictly positive and continuous differentiable ground state. See [43] (Thm.XIII.46 and XIII.47) for the regularities conditions on the potentials V and v implying the strictly positivity and (XIII.11) for those implying the differentiability of the ground state wave function.

We denote by $\hat{X}$ the $3N$-dimensional Nelson's diffusion corresponding to the ground state solution ψ_N^0. It satisfies, in a weak sense, the following SDE

$$d\hat{X}_t = \frac{\nabla^{(N)}\Psi_N^0}{\Psi_N^0}(\hat{X}_t)dt + (\frac{\hbar}{m})^{\frac{1}{2}} d\hat{W}_t, \quad (2.12)$$

where $\nabla^{(N)}$ denotes the $3N$-dimensional gradient and $\hat{W}$ is a $3N$-dimensional standard Brownian Motion. The process $\hat{X}$, sometimes named the *ground state process*, can be seen as a family of N one-particle three-dimensional interacting diffusions $(X_1, \ldots, X_N)$:

$$\begin{aligned} dX_1 &= b_1(\hat{X}_t)dt + dW_t^1 \\ dX_2 &= b_2(\hat{X}_t)dt + dW_t^2 \\ &\quad .... \qquad .... \\ &\quad .... \qquad .... \\ dX_N &= b_N(\hat{X}_t)dt + dW_t^N, \end{aligned} \quad (2.13)$$

where $(b_1, b_2, ..., b_N)$ are the $\mathbb{R}^3$-components of the $\mathbb{R}^{3N}$ vector drift $b(\hat{X}_t) = \frac{\nabla^{(N)}\Psi_N^0}{\Psi_N^0}$.

When Bose-Einstein condensation occurs, the condensate is systematically described by the order parameter $\phi_{GP} \in L^2(\mathbb{R}^3)$, also called wave function of the condensate, which is the minimizer of the Gross-Pitaevskii functional

$$E^{GP}[\phi] = \int (\frac{\hbar^2}{2m}|\nabla\phi(r)|^2 + V(r)|\phi(r)|^2 + g|\phi(r)|^4)d\mathbf{r} \quad (2.14)$$

under the L^2-normalization condition

$$\int_{\mathbb{R}^3} |\phi^{GP}|^2 d\mathbf{r} = 1 \tag{2.15}$$

and where $g > 0$ is a parameter depending on the interaction potential v (see also next assumption h3). Therefore ϕ_{GP} solves the stationary cubic non-linear equation (in this context called Gross-Pitaevskii equation)

$$-\frac{\hbar^2}{2m}\triangle\phi + V\phi + 2g|\phi|^2\phi = \lambda\phi, \tag{2.16}$$

λ denoting the chemical potential. One can prove that ϕ_{GP} is continuously differentiable and strictly positive ([29]).

In [34] the stochastic quantization approach for the system of N interacting Bose particles has been exploited for the first time, in particular studying the relevant consequences of working with a symmetric wave function.

It is proved in [37] that the Stochastic Mechanics of the N-body problem associated to H_N uniquely determines a well defined stochastic process which describes the motion of the single particle in the condensate, in the case of the Gross-Pitaevskii scaling limit as introduced in [29], which allows to prove the existence of an exact Bose-Einstein condensation for the ground state of H^N ([29],[30]).

3. Mean Energy Rescaling and its Asymptotic Behaviour

For simplicity of notations, we will put $\hbar = 2m = 1$.

The main mathematical tool for studying the system of N interacting diffusions is the mean quantum mechanical energy (2.8), with Ψ_N denoting a solution of the Schrödinger equation corresponding to H_N. Putting $\rho_N := |\Psi_N|^2$, the mean energy (2.8) can be expressed in terms of the joint probability density of our $3N-$dimensional process $\hat{X}$ as:

$$E[\rho_N] = E\{\sum_{i=1}^{N}[b_i^2(\hat{X}) + V(X_i(t))] + \sum_{1\le i<j\le N} v(X_i(t) - X_j(t))\} \tag{3.1}$$

b_i being the drift of the interacting i-th particle, whose position is given by the process X_i.

Following [29], we assume

h1) $V(|\mathbf{r_i}|)$ locally bounded, positive and going to infinity when $|\mathbf{r_i}|$ goes to infinity.

h2) v smooth, compactly supported, non negative, spherically symmetric, with finite *scattering length* a ([31] Appendix C).

We perform the following scaling, known as Gross-Pitaevskii (GP) scaling [29], writing

h3)

$$v(r) = v_1(\frac{r}{a})/a^2$$

$$a = \frac{g}{4\pi N}$$

where v_1 has scattering length equal to 1 and remains fixed while $N \uparrow +\infty$. Moreover $g > 0$ as a consequence of our assumptions on v.

In the GP limit the product Na remains fixed: this is experimentally justified since N can be quite large, 10^{11} or more, and Na can vary from 1 to 10^4. Finally, fixing Na means that the limit is a *dilute* one. In fact, being the asymptotic mean density $\hat{\rho} \sim N$, one has that

$$\hat{\rho} a^3 \sim N^{-2} \ll 1$$

i.e. the mean inter-particle distance $\hat{\rho}^{-1/3}$ is much larger than the *scattering length* a. Moreover the GP limit is a *dynamical* one, where the kinetic and potential energies remain comparable ([35]).

In [29] and [30] three important theorems are proven. We denote them as *Energy Theorem*, *Energy Localization Theorem* and *Bose Einstein Condensation Theorem*, and reformulate them with different notations for future convenience.

Theorem 3.1. *(Energy) ([29]) Under the previous hypothesis h1),h2) h3) then*

$$\lim_{N\to\infty} \frac{E[\rho_N^0]}{N} = E[\rho_{GP}] \tag{3.2}$$

and

$$\lim_{N\to\infty} \int \rho_N^0 d\mathbf{r}_2 \cdots d\mathbf{r}_N = \rho_{GP}, \tag{3.3}$$

where $\rho_{GP} := |\phi_{GP}|^2$, with ϕ_{GP} the minimizer of the Gross-Pitaevskii functional (2.14)*, $\rho_N^0 := |\Psi_N^0|^2$, with Ψ_N^0 the ground state of H_N, and the convergence in* (3.3) *is in weak $L^1(\mathbb{R}^3)$ sense.*

Moreover, let ϕ_0 denote the solution of the zero-energy scattering equation for v (i.e. $-\triangle\phi_0(\mathbf{r}) + \frac{1}{2}v(\mathbf{r})\phi_0(\mathbf{r}) = 0$) under the boundary condition $\lim_{|\mathbf{r}|\to+\infty} \phi_0(\mathbf{r}) = 1$ and $s = \int |\nabla\phi_0|^2/(4\pi a)$. Then $s \in (0,1]$ and

$$\begin{aligned}\lim_{N\uparrow\infty} \int_{\mathbb{R}^{3N}} |\nabla_1 \sqrt{\rho_N^0}(\mathbf{r}_1, ..., \mathbf{r}_N)|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N = \int_{\mathbb{R}^3} |\nabla \sqrt{\rho_{GP}}(\mathbf{r})|^2 d\mathbf{r} \\ + gs \int_{\mathbb{R}^3} (\rho_{GP}(\mathbf{r}))^2 d\mathbf{r}\end{aligned} \tag{3.4}$$

$$\lim_{N\uparrow\infty} \int_{\mathbb{R}^{3N}} V(\mathbf{r})\rho_N^0(\mathbf{r}_1, ..., \mathbf{r}_N))d\mathbf{r}_1 \cdots d\mathbf{r}_N = \int V(\mathbf{r})\rho_{GP}(\mathbf{r})d\mathbf{r} \tag{3.5}$$

$$\lim_{N\uparrow\infty} \frac{1}{2} \sum_{j=2}^{N} \int_{\mathbb{R}^{3N}} v(|\mathbf{r}_1 - \mathbf{r}_j|)\rho_N^0(\mathbf{r}_1, ..., \mathbf{r}_N)d\mathbf{r}_1 \cdots d\mathbf{r}_N = (1-s)g \int (\rho_{GP}(\mathbf{r}))^2 d\mathbf{r}. \tag{3.6}$$

The second theorem shows that asymptotically the interaction energy localizes into small balls surrounding each particle.

Theorem 3.2. *(Energy Localization) ([30]). Defining*

$$F^N(\mathbf{r}_2, ..., \mathbf{r}_N) := \left(\bigcup_{i=2}^{N} B^N(\mathbf{r}_i) \right)^c, \tag{3.7}$$

where $()^c$ stands for complement and $B^N(\mathbf{r})$ denotes the open ball centered in $\mathbf{r}$ with radius $N^{-\frac{1}{3}-\delta}$, where $0<\delta\leq\frac{4}{51}$,

$$\lim_{N\uparrow\infty}\int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2\cdots d\mathbf{r}_N\int_{F^N(\mathbf{r}_2,\dots,\mathbf{r}_N)}\left(\frac{\nabla_1\sqrt{\rho_N^0}}{\sqrt{\rho_N^0}}-\frac{\nabla_1\sqrt{\rho_{GP}}}{\sqrt{\rho_{GP}}}\right)^2\rho_N^0 d\mathbf{r_1}=0. \quad (3.8)$$

Theorem 3.1 and Theorem 3.2 are really important because they allow to prove the complete BEC for bosons in a trap ([30]).

The mathematical concept of BEC can be properly formulated in terms of the one-particle density matrix, that is the operator on $L^2(\mathbb{R}^3)$ given by the kernel

$$\gamma(\mathbf{r},\mathbf{r}')=\int\Psi_N(\mathbf{r},\mathbf{r_2},...,\mathbf{r_N})\cdot\Psi_N(\mathbf{r}',\mathbf{r_2},...,\mathbf{r_N})d\mathbf{r_2}\cdots d\mathbf{r_N}. \quad (3.9)$$

Definition 3.3. *Complete* or *exact* BEC is defined to be the property that as $N\uparrow+\infty$

$$\gamma(\mathbf{r},\mathbf{r}')\longrightarrow\phi(\mathbf{r})\cdot\phi(\mathbf{r}') \quad (3.10)$$

in some topology for density matrices.

Under the hypothesis h1),h2),h3), the following relevant theorem is proved in [30].

Theorem 3.4. *(BEC) For each fixed Na*

$$\lim_{N\uparrow+\infty}\gamma(\mathbf{r},\mathbf{r}')=\sqrt{\rho_{GP}(\mathbf{r})}\cdot\sqrt{\rho_{GP}(\mathbf{r}')} \quad (3.11)$$

in trace norm and in $L^2(\mathbb{R}^3\times\mathbb{R}^3)$.

Proposition 3.5. *BEC Theorem implies the complete condensation for all n-particle reduced density matrices ($n\geq1$), i.e.*

$$\lim_{N\uparrow+\infty}\gamma^n(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_n,\mathbf{r}'_1,\mathbf{r}'_2,...,\mathbf{r}'_n)=$$
$$\sqrt{\rho_{GP}(\mathbf{r_1})}\cdot\sqrt{\rho_{GP}(\mathbf{r_1'})}\cdots\sqrt{\rho_{GP}(\mathbf{r_n})}\cdot\sqrt{\rho_{GP}(\mathbf{r_n'})} \quad (3.12)$$

where the convergence is in the same sense of Theorem 3.4.

The proof of Proposition 3.5 in [30] takes advantage of the second quantization formalism. See [35] for an alternative proof in L^2 spaces.

4. A Transition to Chaos Result

We illustrate a rigorous probabilistic counterpart, in the frame of Nelson's Stochastic Mechanics, of the three important quantum theorems we recalled in section 3.

We firstly observe that the fixed time joint probability density of $(X_1,...,X_N)$ is given by $\rho_N^0:=|\Psi_N^0|^2$, which is invariant under spatial permutations. In [37] it has been proved that if Ψ_N^0 is the ground state of H_N and it is strictly positive and of class C^1, then the three-dimensional processes $\{X_i\}_{i=1,\dots,N}$ are equal in law.

From Proposition 3.5 we can derive the following

Corollary 4.1. *For $N \uparrow +\infty$ the n-particle marginal density ($n \geq 1$)*

$$\rho_N^{(n)} := \int \rho_N d\mathbf{r_{n+1}} \cdots d\mathbf{r_N} \tag{4.1}$$

is such that

$$\lim_{N\uparrow+\infty} \rho_N^{(n)} = \rho_{GP}^{\otimes n} \tag{4.2}$$

in the weak convergence sense.

Proof. We take $n = 1$ for simplicity. From Proposition 3.5 we have that when $N \uparrow \infty$

$$\int\int (\gamma(\mathbf{r},\mathbf{r'}) - \sqrt{\rho_{GP}(\mathbf{r})} \cdot \sqrt{\rho_{GP}(\mathbf{r'})})^2 d\mathbf{r}d\mathbf{r'} \longrightarrow 0. \tag{4.3}$$

Let us now reduce to the diagonal of the n-particle reduced density kernel γ. Ψ_N^0 being continuous, this is meaningful (see [35] for a summary on technical results about the reduction to the diagonal).

We obtain that when $N \uparrow \infty$

$$\int (\rho_N^{(1)}(\mathbf{r}) - \rho_{GP}(\mathbf{r}))^2 d\mathbf{r} \longrightarrow 0. \tag{4.4}$$

By Schwarz inequality for all $\phi \in C_b(\mathbb{R}^3)$

$$|\int \phi(\rho_N^{(1)} - \rho_{GP})|d\mathbf{r} \leq \|\phi\|_2 \|\rho_N^{(1)} - \rho_{GP}\|_2 \tag{4.5}$$

(with $\|\cdot\|_2$ the L^2-norm), i.e. the probability density $\rho_N^{(1)}$ converges weakly to the probability density ρ_{GP}. The proof is the same for $n > 1$. For example $\rho_N^{(2)}(\mathbf{r_1},\mathbf{r_2})$ converges weakly to $\rho_{GP}(\mathbf{r_1}) \cdot \rho_{GP}(\mathbf{r_2})$, etc. $\square$

Putting now $E = \mathbb{R}^3$, let $\mathbf{v}_N$ be the probability measures on E^N having density ρ_N^0 and let $\mathbf{v}_{GP}$ be the probability measure on E having density ρ_{GP} with respect to the Lebesgue measure.

With the usual notation

$$< \mu, \phi >= \int \phi(x)\mu(dx) \tag{4.6}$$

for a probability measure μ on E and $\phi \in C_b(E)$, we recall the following

Definition 4.2. ([45]). Let E be a separable metric space, $\mathbf{u}_N$ a sequence of symmetric probability measures on E^N. We say that $\mathbf{u}_N$ is $\mathbf{u}-$ *chaotic*, $\mathbf{u}$ a probability measure on E, if for $\phi_1, \phi_2, ..., \phi_n \in C_b(E)$

$$\lim_{N\uparrow+\infty} < \mathbf{u}_N, \phi_1 \otimes \phi_2 \otimes ... \otimes \phi_n \otimes 1 \cdots 1 >= \prod_{i=1}^{n} < \mathbf{u}, \phi_i > . \tag{4.7}$$

The above definition can be reformulated by considering the standard projection map of the $\mathbf{u}_N$ on E^n and saying that the projection converges to $\mathbf{u}^{\otimes n}$ when N goes to $+\infty$ ([5], p.20).

Therefore, Proposition 3.5 and Corollary 4.1 allow to prove the following:

Proposition 4.3. *Under the hypothesis h1),h2),h3), the probability measures* $\mathbf{v}_N$*, uniquely associated to the Hamiltonian* H_N *through the relation* $\rho_N^0 = |\Psi_N^0|^2$*,* Ψ_N^0 *denoting the ground state of* H_N*, is* $\mathbf{v}_{GP}$*-chaotic according with the above Definition 4.2.*

Let us now introduce, for N fixed, the so called *empirical measure* (see for example [8])

$$X_N(t) := \frac{\sum_{i=1}^N \delta_{X_i(t)}}{N}. \tag{4.8}$$

where for all i: $\delta_{X_i(t)}$ is a random measure on $\mathcal{B}(\mathbb{R}^3)$ such that, for all $\phi \in C_0(\mathbb{R}^3)$

$$\int \phi(x)\delta_{X_i(t)}(dx) = \phi(X_i(t)). \tag{4.9}$$

Therefore, finally, the *empirical measure* is such that for all $\phi \in C_0(\mathbb{R}^3)$

$$\int \phi(x)[X_N(t)](dx) = \frac{\sum_{i=1}^N \phi(X_i(t))}{N}. \tag{4.10}$$

In particular, for $A \in \mathcal{B}(\mathbb{R}^3)$

$$[X_N(t)](A) := \frac{\sharp\{X_i(t) \in A\}}{N} \tag{4.11}$$

i.e. the *empirical measure* of a set A is the relative frequency of particles which stay in A at time t.

One can easily prove the following ([45])

Proposition 4.4. *The two statements are equivalent:*

a) $\mathbf{v}_N$ *is* $\mathbf{v}_{GP}$*-chaotic.*

b) $X_N(t) = \frac{\sum_{i=1}^N \delta_{X_i(t)}}{N}$ *converge in law to the constant random variable* $\mathbf{v}_{GP}$*.*

Proof. We report for completeness the implication a)$\Longrightarrow$ b) (for the other implication see [45])

Let us suppose that (4.7) is true for $n = 1, 2$, i.e.

$$\lim_{N\uparrow+\infty} \int \phi_1(\mathbf{r}_1)\rho_N^{(1)}(\mathbf{r}_1)d\mathbf{r}_1 = \int \phi_1(\mathbf{r}_1)\rho_{GP}(\mathbf{r}_1)d\mathbf{r}_1, \tag{4.12}$$

$$\lim_{N\uparrow+\infty} \int \phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)\rho_N^{(2)}(\mathbf{r}_1, \mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2 = [\int \phi(\mathbf{r}_1)\rho_{GP}(\mathbf{r}_1)d\mathbf{r}_1)]^{\otimes 2}, \tag{4.13}$$

with $\phi_1, \phi_2 \in C_b(E)$. Taking $\phi \in C_b(E)$ one has:

$$
\begin{aligned}
E_{\rho_N^0}[(< X_N - \mathbf{v}_{GP}, \phi >)^2] &= E_{\rho_N^0}[(< X_N, \phi >)^2] + (< \mathbf{v}_{GP}, \phi >)^2 \\
&\quad - 2 < \mathbf{v}_{GP}, \phi > E_{\rho_N^0}[< X_N, \phi >] \\
&= E_{\rho_N^0}[(\frac{\sum_{i=1}^N \phi(X_i)}{N})^2] + (< \mathbf{v}_{GP}, \phi >)^2 - 2 < \mathbf{v}_{GP}, \phi > E_{\rho_N^0}[\frac{\sum_{i=1}^N \phi(X_i)}{N}] \\
&= \frac{1}{N^2}\{N E_{\rho_N^0}[(\phi(X_1))^2] + N(N-1)E_{\rho_N^0}[\phi(X_1)\cdot\phi(X_2)]\} + (< \mathbf{v}_{GP}, \phi >)^2 \\
&\quad - 2 < \mathbf{v}_{GP}, \phi > E_{\rho_N^0}[\phi(X_1)] \\
&= \frac{1}{N}\int (\phi(\mathbf{r}_1))^2 \rho_N^{(1)}(\mathbf{r}_1) d\mathbf{r}_1 + \frac{N-1}{N}\int \phi(\mathbf{r}_1)\cdot\phi(\mathbf{r}_2)\rho_N^{(2)}(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2 \\
&\quad + (< \mathbf{v}_{GP}, \phi >)^2 - 2 < \mathbf{v}_{GP}, \phi > \int \phi(\mathbf{r}_1))^2 \rho_N^{(1)}(\mathbf{r}_1) d\mathbf{r}_1, \quad (4.14)
\end{aligned}
$$

where the symmetry of ρ_N^0 has been exploited. Sending $N \uparrow +\infty$ and using the hypothesis one obtains b). □

The statement b) is a sort of law of large numbers. When N is finite the random variables X_i are far from being independent, but asymptotically the N particles behave *as* they were independent. In fact Corollary 4.1 says that the any finite dimensional distribution of $\hat{X}$ factorizes in the limit. This is the meaning of the phrase: *a transition to chaos*, where *chaos* stays for *independence*.

In the BEC regime a single particle feels the interaction only when it arrives *very very* near to another particle, as the *Energy Localization Theorem* points out. Before that time it does not feel the interaction. From the probabilistic point of view we recognize in the BEC regime a *Poisson approximation* one.

In the next section we will get a little more inside this stochastic picture.

5. One Particle Relative Entropy

In this section the results contained in [37] and in [39] are briefly exposed. The *Energy Theorem* says that the one-particle marginal density of ρ_N^0 converges to ρ_{GP} in the weak $L^1(\mathbb{R}^3)$ sense. So we introduce a process X^{GP} with invariant measure $\rho_{GP} d\mathbf{r}$ and try to compare it with the generic interacting *non* markovian diffusion $X_1(t)$ ([34]).

We assume that X^{GP} is a solution of the SDE

$$dX_t^{GP} := u_{GP}(X_t^{GP})dt + (\frac{\hbar}{m})^{\frac{1}{2}} dW_t, \qquad (5.1)$$

where,

$$u_{GP} := \frac{1}{2}\frac{\nabla \rho_{GP}}{\rho_{GP}}. \qquad (5.2)$$

We now try to compute the distance in relative entropy between the three-dimensional one-particle non markovian diffusion X_1 and X^{GP}. To this extent we introduce a $3N$-dimensional process $\hat{X}^{GP}$ which satisfies a stochastic differential equation with the same diffusion coefficient as $\hat{X}$ and drift $\hat{u}_{GP}$, defined by

$$\hat{u}_{GP}(\mathbf{r}_1, \cdots, \mathbf{r}_N) = (u_{GP}(\mathbf{r}_1), \cdots, u_{GP}(\mathbf{r}_N)). \qquad (5.3)$$

We consider the measurable space $(\Omega^N, \mathcal{F}^N)$ where Ω^N is $C(\mathbb{R}^+ \to \mathbb{R}^{3N})$, and $\mathcal{F}^N$ is its Borel sigma-algebra. We denote by $\hat{Y} := (Y_1, \dots, Y_N)$ the coordinate process and by $\mathcal{F}_t^N$ the natural filtration.

We denote by $\mathbb{P}_N$ and $\mathbb{P}_{GP}$ the measures corresponding to the weak solutions of the $3N$- dimensional stochastic differential equations

$$\hat{Y}_t - \hat{X}_0 = \int_0^t \hat{b}^N(\hat{Y}_s)ds + \hat{W}_t, \tag{5.4}$$

$$\hat{Y}_t - \hat{X}_0 = \int_0^t \hat{u}_{GP}(\hat{Y}_s)ds + \hat{W}'_t, \tag{5.5}$$

where $\hat{X}_0$ is a random variable with probability density equal to ρ_N^0, while $\hat{W}_t$ and $\hat{W}'_t$ are $3N$-dimensional $\mathbb{P}_N$ and $\mathbb{P}_{GP}$ standard Brownian Motions, respectively.

In this section we use the shorthand notation

$$\hat{b}_s^N =: \hat{b}^N(\hat{Y}_s), \quad \hat{u}_s^N =: \hat{u}_{GP}(\hat{Y}_s).$$

In order to use Girsanov Theorem, we will assume that u_{GP} is bounded. We recall that under our hypothesis on the potentials v and V, ρ_{GP} is strictly positive and in $C^1(\mathbb{R}^3) \bigcap L^\infty(\mathbb{R}^3)$ and therefore $u_{GP} \in L^2(\mathbb{R}^3)$ (see [29], Thm 2.1). Then the following finite energy conditions hold:

$$E_{\mathbb{P}_N} \int_0^t \|\hat{b}_s^N\|^2 ds < \infty, \tag{5.6}$$

$$E_{\mathbb{P}_N} \int_0^t \|\ \hat{u}_s^{GP}\|^2 ds < \infty, \tag{5.7}$$

which follow from the fact that Ψ_N^0 is the minimizer of $E^N[\Psi]$, and our hypothesis on u_{GP}.

Then, by Girsanov's theorem, we have, for all $t > 0$,

$$\frac{d\mathbb{P}_N}{d\mathbb{P}_{GP}}|_{\mathcal{F}_t} = \exp\{-\int_0^t (\hat{b}_s^N - \hat{u}_s^{GP}) \cdot d\hat{W}_s + \frac{1}{2}\int_0^t \|\hat{b}_s^N - \hat{u}_s^{GP}\|^2 ds\}, \tag{5.8}$$

where $|.|$ denotes the Euclidean norm in $\mathbb{R}^{3N}$. The relative entropy restricted to $\mathcal{F}_t$ reads

$$\mathcal{H}(\mathbb{P}_N, \mathbb{P}_{GP})|_{\mathcal{F}_t} \ =: \ \mathbb{E}_{\mathbb{P}_N}[\log \frac{d\mathbb{P}_N}{d\mathbb{P}_{GP}} \ \ |_{\mathcal{F}_t}] \ = \ \frac{1}{2} E_{\mathbb{P}_N} \int_0^t \|\hat{b}_s^N \ - \ \hat{u}_s^{GP}\|^2 ds. \tag{5.9}$$

Since under $\mathbb{P}_N$ the $3N$-dimensional process $\hat{Y}$ is a solution of (5.4) with invariant probability density ρ_N^0 , we can write, recalling also (5.6) and (5.7),

$$\begin{aligned}
&\frac{1}{2} E_{\mathbb{P}^N} \int_0^t \|\hat{b}_s^N - \hat{u}_s^{GP}\|^2 ds \\
&\qquad = \frac{1}{2}\int_0^t E_{\mathbb{P}_N} \|\hat{b}_s^N - \hat{u}_s^{GP}\|^2 ds \\
&\qquad = \frac{1}{2} t \int_{\mathbb{R}^{3N}} \|\hat{b}^N(\mathbf{r}_1, \dots, \mathbf{r}_N) - \hat{u}_{GP}(\mathbf{r}_1, \dots, \mathbf{r}_N)\|^2 \rho_N^0 d\mathbf{r}_1 \dots d\mathbf{r}_N.
\end{aligned} \tag{5.10}$$

so that we get

$$\begin{aligned}
&\mathcal{H}(\mathbb{P}_N, \mathbb{P}_{GP})|_{\mathcal{F}_t} \\
&= \frac{1}{2}t\int_{\mathbb{R}^{3N}} \sum_{i=1}^{N} \|b_i^N(\mathbf{r}_1,\dots,\mathbf{r}_N) - u_{GP}(\mathbf{r}_i)\|^2 \rho_N^0 d\mathbf{r}_1 \dots d\mathbf{r}_N \\
&= \frac{1}{2}Nt\int_{\mathbb{R}^{3N}} \|b_1^N(\mathbf{r}_1,\dots,\mathbf{r}_N) - u_{GP}(\mathbf{r}_1)\|^2 \rho_N^0 d\mathbf{r}_1 \dots d\mathbf{r}_N \\
&= \frac{1}{2}NE_{\mathbb{P}_N}\int_0^t \|b_1^N(\hat{Y}_s) - u_{GP}(Y_1(s))\|^2 ds, \qquad (5.11)
\end{aligned}$$

where the symmetry of $\hat{b}^N$ and ρ_N^0 has been exploited.

Finally we get the sum of N identical *one-particle relative entropies*, each of them being defined by

$$\begin{aligned}
\bar{\mathcal{H}}(\mathbb{P}_N, \mathbb{P}_{GP})|_{\mathcal{F}_t} &=: \frac{1}{N}\mathcal{H}(\mathbb{P}_N, \mathbb{P}_{GP})|_{\mathcal{F}_t} \\
&= \frac{1}{2}E_{\mathbb{P}_N}\int_0^t \|b_1^N(\hat{Y}_s) - u^{GP}(Y_1(s))\|^2 ds. \qquad (5.12)
\end{aligned}$$

By the *Energy Theorem* we can deduce that for any $t > 0$ the one particle relative entropy is asymptotically *finite* but it does not go to zero in the scaling limit.

On the other hand, the relevant *Energy Localization Theorem* now says that the asymptotic *finite* relative entropy, between the one particle process and the GP process, is supported only on smaller and smaller balls surrounding each particle ([39]).

In fact, the thesis of the *Energy Localization Theorem* can be now read

$$\lim_{N\uparrow\infty}\int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2\cdots d\mathbf{r}_N \int_{F^N(\mathbf{r}_2,\dots,\mathbf{r}_N))} \|b_1^N - u_{GP}\|^2 \rho_N^0 d\mathbf{r}_1 = 0. \qquad (5.13)$$

Let us finally introduce the following time dependent random subset of $\mathbb{R}^3$

$$D_N(t) := \bigcup_{i=2}^{N} B^N(X_i(t)) \qquad (5.14)$$

where $B^N(\mathbf{r})$ is again the ball with radius $N^{-1/3-\delta}$, $\quad 0 < \delta \leq 4/51$, centered in $\mathbf{r}$, and the stopping time

$$\tau^N := inf\{t \geq 0 : X_1(t) \in D_N(t)\} \qquad (5.15)$$

We explore the possibility that, for large N, the one particle process continuously *lives* outside the interaction-set $D_N(t)$ the most part of the time, and that the τ^N- stopped version of X_1 converges in some sense to the τ^N-stopped version of X^{GP}.

Notice that this conjecture is not obvious. In fact, even in dimension $d = 3$, where the Lebesgue measure of $D_N(t)$ goes to zero for all t, it could happen that, asymptotically as N goes to infinity, such a set takes the form of a very complicated surface, dividing the physical three-dimensional space into smaller and smaller non connected regions. On the other hand we are dealing with a random system, so that it could happen that the probability of such an event is equal to zero.

The following proposition, which affirms that, in the scaling limit, a generic particle remains outside the *interaction-set*, for any finite time interval, with probability one, has been proved in [37]

Proposition 5.1. *Let $h1), h2)$ and $h3)$ hold and the ground state Ψ_N^0 be of class C^1. Then in dimension $d = 3$, for all $t > 0$, we have*

$$\lim_{N\to\infty} \mathbb{P}(\tau^N > t \mid X_1(0) \notin D_N(0)) = 1 \tag{5.16}$$

and τ^N has an exponential distribution.

Finally if we consider the stopped one-particle process, for it we can prove its convergence to the GP process in the relative entropy sense exploiting the *Energy Localization Theorem* (see also [37])

Proposition 5.2. *Let $h_1)$ $h_2)$ and $h_3)$ hold. Assume also that Ψ_N^0 is of class C^1 and that u_{GP} is bounded. Then, with τ^N defined as in (5.15), we have*

$$\lim_{N\uparrow\infty} \bar{\mathcal{H}}(\mathbb{P}_N, \mathbb{P}_{GP}) \mid_{\mathcal{F}_{t\wedge\tau^N}} = 0 \tag{5.17}$$

Proof. Recalling (5.6) and (5.7) we can write

$$\begin{aligned}
&\bar{\mathcal{H}}(\mathbb{P}_N, \mathbb{P}_{GP})|_{\mathcal{F}_{t\wedge\tau^N}} = \frac{1}{2}E_{\mathbb{P}_N}\int_0^{t\wedge\tau^N} \|b_1^N(\hat{Y}_s) - u_{GP}(Y_1(s))\|^2 ds\\
&\le \frac{1}{2}\int_0^t E_{\mathbb{P}_N}\{\|b_1^N(\hat{Y}_s) - u_{GP}(Y_1(s))\|^2 I_{\{Y_1\notin D_s^N\}}\}ds\\
&= \frac{1}{2}tE_{\mathbb{P}_N}\{\|b_1^N(\hat{Y}_s) - u_{GP}(Y_1(s))\|^2 I_{\{Y_1\notin D_s^N\}}\}\\
&= \frac{1}{2}t\int_{\mathbb{R}^{3N}} \|b_1^N(\mathbf{r}_1,\ldots,\mathbf{r}_N) - u_{GP}(\mathbf{r}_1)\|^2 I_{F^N(\mathbf{r}_2,\ldots,\mathbf{r}_N)}\quad(\mathbf{r}_1)\rho_N^0 d\mathbf{r}_1\cdots d\mathbf{r}_N.
\end{aligned} \tag{5.18}$$

Recalling (5.13), we finally get

$$\begin{aligned}
&\lim_{N\uparrow\infty} \bar{\mathcal{H}}(\mathbb{P}_N, \mathbb{P}_{GP})|_{\mathcal{F}_{t\wedge\tau^N}}\\
&\quad= \frac{1}{2}t\lim_{N\uparrow\infty}\int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2\ldots d\mathbf{r}_N \int_{F^N(\mathbf{r}_2,\ldots,\mathbf{r}_N)} \|b_1^N - u_{GP}\|^2\rho_N^0 d\mathbf{r}_1\cdots d\mathbf{r}_N\\
&\quad= 0.
\end{aligned} \tag{5.19}$$

□

6. APPENDIX

The proofs of the *Energy* and *Energy Localization* theorems are very similar and substantially devoted to establish a lower bound for an energy form. In order to establish the *Energy Theorem* it is also necessary to derive an upper bound for $E[\rho_N^0]$. But this is much easier (see [31] pag.52).

The proof of the lower bound is essentially based on two fundamental results regarding the following interacting Hamiltonian

$$H_N^I = -\sum_{i=1}^{N} \Delta_i + \sum_{1 \leq i \leq j \leq N} v(|x_i - x_j|) \tag{6.1}$$

for N bosons in a cubic box of side length L, corresponding to the density *homogeneous case*.

The first result is a generalization of a Dyson's Lemma ([15]) by Lieb and Yngvason ([32]), which we report in a simplified version:

Lemma 6.1. *(Smoothing Lemma) Let $v(r) \geq 0$ with finite range R_0 and let $U(r) \geq 0$ be any function satisfying*

$$\int U(r) r^2 dr \leq 1 \qquad U(r) = 0 \quad r < R_0 \tag{6.2}$$

Then

$$E\{\sum_{i=1}^{N} [b_i^2(\hat{X})] + \sum_{1 \leq i < j \leq N} v(X_i(t) - X_j(t))\} \geq E\{\sum_{i=1}^{N} \epsilon b_i^2(\hat{X}) + a(1-\epsilon) U(S_i)\} \tag{6.3}$$

where

$$S_i := \min_{j, j \neq i} |X_i - X_j| \tag{6.4}$$

denotes the position of the nearest particle to particle i and the integration domain in (6.3) *is any convex subset of $\mathbb{R}^3$ containing the zero.*

Remark 6.2. a) One can take

$$U(r) = 3(R^3 - R_0^3)^{-1} \qquad R_0 < r < R \tag{6.5}$$

and otherwise equal to zero, where R represents the range of the potential U substituting the interaction potential v having range R_0.

b) The *Smoothing Lemma* substitutes a very soft and nearest-neighbor potential for the original pair interacting potential v at the price of sacrificing some part of the kinetic energy ([31]). This is equivalent to saying that moving towards a low particles density region, where the strength of the Brownian noise is attenuated and the single particle feels only its nearest neighbor, can only lower the mean energy.

The second fundamental result is the following estimate for the density *homogeneous case* due to Lieb and Yngvason ([32])

Theorem 6.3. *(Lower bound Theorem LBT) Let* (6.1) *be the Hamiltonian for N interacting bosons in a cubic box Λ with side length L, where v is a spherically symmetric pairs potential having finite scattering length a. Then there exists a $\lambda > 0$ such that the ground state energy of H_N^I, with Neumann boundary conditions, satisfies*

$$\frac{E_0[\rho_N^0]}{N} \geq 4\pi\rho a(1 - CY^{1/17}) \tag{6.6}$$

where $\rho = \frac{N}{L^3}$ is the fixed particle density and $Y = 4\pi\rho\frac{a^3}{3}$ is the number of particles in the ball of radius a, for all N and L such that $Y < \lambda$ and $\frac{L}{a} > C_1 y^{-\frac{6}{17}}$. Moreover C and C_1 are positive constants independent of N and L.

Proof. (**Sketch of the proof of the LBT**) (see [31] Theorem 2.4, p.18) Because of $Y < \lambda$ the estimate is true in a low particles density regime. The condition on $\frac{L}{a}$ implies $N \geq C_2 Y^{-1/17}$. Starting from the right hand side of (6.3), approaching the operator $-\epsilon\triangle + a(1-\epsilon)U$ by the point of view of first order perturbation theory and applying the cell-method (the big box Λ is divided into cubic *cells* of side length l that it is kept fixed as $L \uparrow +\infty$) the authors of [31] establish the following lower bound

$$\frac{E_0[\rho_N^0]}{N} \geq 4\pi\rho a(1 - \frac{1}{\rho l^3})K(4\rho l^3, l), \tag{6.7}$$

where

$$\begin{aligned} K(4\rho l^3, l) \geq (1-\epsilon)(1 - \frac{2R}{l})^3(1 + C_1 Y(\frac{l}{a})^3(\frac{R^3 - R_0^3)}{l^3})^{-1} \\ \times (1 - \frac{l^3}{R^3 - R_0^3}\frac{C_2 Y}{(\epsilon(a/l)^2 - C_3 Y^2(l/a)^3)}) \end{aligned} \tag{6.8}$$

with $Y = 4\pi\rho\frac{a^3}{3}$. Since there is no convexity of the ground state energy before having reached the limit, they take advantage of the *superadditivity* property of E_0 in order to obtain that $n = O(\rho l^3)$ in all boxes.

With the ansatz

$$\epsilon \sim Y^\alpha, \quad a/l \sim Y^\beta, \quad (R^3 - R_0^3)/l^3) \sim Y^\gamma \tag{6.9}$$

the following choice

$$\alpha = 1/17, \quad \beta = 6/17, \quad \gamma = 3/17 \tag{6.10}$$

implies the validity of (6.7).

This choice means in particular that

$$a \ll R \ll \rho^{-\frac{1}{3}} \tag{6.11}$$

where R is the range of the near neighbors potential U. □

Proof. (**Energy Theorem**)(see [31], Theorem 6.2) We only prove the convergence of the energies (3.2). The density convergence follows easily in the usual way by variation with respect to the external potential and (3.4),(3.5) and (3.6) can be obtained by (3.2) by variation with respect to the different components of the energy, as noted in [11].

If Ψ_N is a general wave function, let us put $\rho_N = |\Psi_N|^2$ and

$$\sqrt{\rho_N} = \prod_{k=1}^{N} \sqrt{\rho_{GP}(\mathbf{r}_k)} \cdot F(r_1, r_2, ...r_N) \tag{6.12}$$

Integrating by part and using the GP variational equation (2.16) for ϕ_{GP}, one can write:

$$\frac{E[\rho_N]}{N} - E[\rho_{GP}] = 4\pi Na \int \rho_{GP}^2 dr + \frac{Q(F)}{N} \tag{6.13}$$

where

$$Q(F) = E_{\rho_N}\{\sum_{i=1}^{N} |\frac{\nabla_i F}{F}|^2 + [\frac{1}{2}\sum_{j\neq i} v(|X_i - X_j|) - 8\pi N a \rho_{GP}(X_i)]\} \tag{6.14}$$

We note that:

$$\frac{\nabla_i F}{F} = \frac{\nabla_i \sqrt{\rho_N}}{\sqrt{\rho_N}} - \frac{\nabla_i \sqrt{\rho_{GP}}}{\sqrt{\rho_{GP}}} \tag{6.15}$$

Minimizing $Q(F)$ we will show that when $N \uparrow +\infty$

$$\frac{Q(F)}{N} \geq -4\pi N a \int \rho_{GP}^2(\mathbf{r}) d\mathbf{r} + o(1) \tag{6.16}$$

implying by (6.13) the convergence of the energies with $E[\rho_N] = E_0[\rho_N^0]$.

Following [31] we minimize $Q(F)$ using the cell-method, taking advantage in each cell of the estimate given for the homogeneous case by the LBT. Successively we minimize over all possible distributions of the particles in the different cells. Since we are looking for a lower bound and the interaction potential v is positive, we can ignore the interactions among the particles in different cells. Finally we take the cell dimension going to zero.

Labeling the cell with the index α, one has

$$\inf_F Q(F) \geq \inf_{n_\alpha} \sum_\alpha \inf_{F_\alpha} Q^\alpha(F_\alpha)$$

where Q^α is defined as Q but with the integrations limited to the cell α, F_α is the function F with particle number n_α and the infimum is taken over all possible distributions of the particles such that $\sum_\alpha n_\alpha = N$.

We now fixe some $M > 0$ and restrict ourselves to cells inside a cube Λ_M of side length M. In the cells inside Λ_M one can evaluate the maximum and minimum value of ρ_{GP} in the cell α, denoted by $\rho_{\alpha,max}$ and $\rho_{\alpha,min}$ respectively.
For all $1 \leq i \leq n_\alpha$, defining

$$\rho_{n_\alpha}^{(i)}(\mathbf{r}_1, ..., \mathbf{r}_{n_\alpha}) = \prod_{k=1,k\neq i}^{n_\alpha} \rho^{GP}(\mathbf{r}_k)|F_\alpha(\mathbf{r}_1, ..., \mathbf{r}_{n_\alpha})|^2 \tag{6.17}$$

one has

$$\begin{aligned}
&E_{\rho_{n_\alpha}}\{|\frac{\nabla_i F_\alpha}{F_\alpha}|^2 + \frac{1}{2}\sum_{j\neq i} v(|X_i - X_j|)\} \\
&\quad = \int [|\frac{\nabla_i F_\alpha}{F_\alpha}|^2 + \frac{1}{2}\sum_{j\neq i} v(|\mathbf{r}_i - \mathbf{r}_j|)] \prod_{k=1}^{n_\alpha} \rho^{GP}(\mathbf{r}_k)|F_\alpha|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_{n_\alpha} \\
&\quad = \int \rho_{GP}(\mathbf{r}_i)[|\frac{\nabla_i F_\alpha}{F_\alpha}|^2 + \frac{1}{2}\sum_{j\neq i} v(|\mathbf{r}_i - \mathbf{r}_j|)]\rho_{n_\alpha}^{(i)} d\mathbf{r}_1 \cdots d\mathbf{r}_{n_\alpha} \qquad (6.18)
\end{aligned}$$

$$\geq \rho_{\alpha,min} E_{\rho_{n_\alpha}^{(i)}}\{|\frac{\nabla_i \sqrt{\rho_{n_\alpha}^{(i)}}}{\sqrt{\rho_{n_\alpha}^{(i)}}}|^2 + \frac{1}{2}\sum_{j\neq i} v(|X_i - X_j|)\}, \tag{6.19}$$

where the equality $\nabla_i \sqrt{\rho_{n_\alpha}^{(i)}} = \prod_{k=1,k\neq i}^{n_\alpha} \sqrt{\rho^{GP}(\mathbf{r}_k)} \cdot \nabla_i F_\alpha$ has been used.

Now applying the *Smoothing Lemma* to the expectation in (6.19) one has for all $0 \leq \epsilon < 1$ that the right hand side of (6.19) is larger or equal to

$$\rho_{\alpha,min} E_{\rho^{(i)}_{n_\alpha}} \{\epsilon |\frac{\nabla_i \sqrt{\rho^{(i)}_{n_\alpha}}}{\sqrt{\rho^{(i)}_{n_\alpha}}}|^2 + a(1-\epsilon)U(S_i)\} \tag{6.20}$$

Since $\sqrt{\rho_{n_\alpha}} = \sqrt{\rho_{GP}(\mathbf{r}_i)} \cdot \sqrt{\rho^{(i)}_{n_\alpha}}$ one can estimate

$$|\nabla_i \sqrt{\rho_{n_\alpha}}|^2 \leq 2\rho_{\alpha,max} |\nabla_i \sqrt{\rho^{(i)}_{n_\alpha}}|^2 + 2\rho^{(i)}_{n_\alpha} C_M \tag{6.21}$$

with $C_M = \sup_{\mathbf{r}\in\Lambda_M} |\nabla \sqrt{\rho_{GP}}(\mathbf{r})|^2$ independent of N.

Substituting (6.21) into (6.20), summing over i from 1 to n_α and using $\rho_{GP}(\mathbf{r}_i) \leq \rho_{\alpha,max}$ in the expectation we finally get

$$\begin{aligned} Q^\alpha(F_\alpha) \geq \frac{\rho_{\alpha,min}}{\rho_{\alpha,max}} \sum_{i=1}^{n_\alpha} E_{\rho_{n_\alpha}} \{\frac{\epsilon}{2} |\frac{\nabla_i \sqrt{\rho_{n_\alpha}}}{\sqrt{\rho_{n_\alpha}}}|^2 + a(1-\epsilon)U(S_i)\} \\ - 8\pi N a \rho_{\alpha,max} n_\alpha - \epsilon C_M n_\alpha. \end{aligned} \tag{6.22}$$

In order to minimize (6.22) with respect to n_α we can use the *Lower Bound Theorem* on the box α having side length L

$$E_0(n_\alpha, L) := \sum_{i=1}^{n_\alpha} E_{\rho^0_{n_\alpha}} \{\frac{\epsilon}{2} |\frac{\nabla_i \sqrt{\rho_{n_\alpha}}}{\sqrt{\rho_{n_\alpha}}}|^2 + a(1-\epsilon)U(S_i)\} \geq n_\alpha \cdot 4\pi a \frac{n_\alpha}{L^3}(1 - CY_\alpha^{\frac{1}{17}}) \tag{6.23}$$

with $Y_\alpha = \frac{a^3 n_\alpha}{L^3}$, provided Y_α is small enough, $\epsilon \geq Y_\alpha^{1/17}$, $n_\alpha \geq C_3 Y_\alpha^{-1/17}$ and $\frac{2R}{L} \sim Y_\alpha^{1/17}$. The condition on ϵ is verified if we choose $\epsilon = Y^{1/17}$ with $Y = \frac{a^3 N}{L^3}$. Ignoring for the moment the last term in (6.22), if $\bar{n}_\alpha$ denotes the value which minimizes the right side of (6.22), then one necessarily has

$$\frac{\rho_{\alpha,min}}{\rho_{\alpha,max}} (E(\bar{n}_\alpha + 1, L) - E(\bar{n}_\alpha, L)) \geq 8\pi a N \rho_{\alpha,max} \tag{6.24}$$

On the other hand, one can prove ([31],p.55, Lemma 6.4) the following

$$E(\bar{n}_\alpha + 1, L) - E(\bar{n}_\alpha, L) \leq 8\pi a \frac{n_\alpha}{L^3} \tag{6.25}$$

Putting together the last two relations one recovers that $\bar{n}_\alpha$ is at least $\sim NL^3$. If one takes $L \sim N^{-1/10}$ then the conditions in order that (6.23) is true are fulfilled for N large enough, i.e.

$$\bar{n}_\alpha \sim N \cdot N^{-3/10} \sim N^{7/10} \tag{6.26}$$

and

$$Y_\alpha = \frac{a^3 \bar{n}_\alpha}{L^3} \sim N^{-3} N^{7/10} N^{3/10} \sim N^{-2} \tag{6.27}$$

where it has been used that $a \sim N^{-1}$. Moreover

$$Y = \frac{a^3 N}{L^3} \sim N^{-7/10}$$

Assuming that n_α is real and dropping the condition $\sum n_\alpha = N$, one can finally minimize

$$4\pi a(\frac{\rho_{\alpha,min}}{\rho_{\alpha,max}}\frac{n_\alpha^2}{L^3}(1-CY^{1/17}) - 2Nn_\alpha\rho_{\alpha,max}), \tag{6.28}$$

finding that the minimum is obtained for

$$\bar{n}_\alpha = N\frac{\rho_{\alpha,max}^2}{\rho_{\alpha,min}}\frac{L^3}{(1-CY^{1/17})} \tag{6.29}$$

Substituting this value of n_α in (6.23), collecting the last term in (6.22) and adding also the contribution of the cells outside Λ_M one can finally write

$$\begin{aligned}\frac{\sum_\alpha Q^\alpha(F_\alpha)}{N} \geq -4\pi Na \sum_{\alpha\subset\Lambda_M} \rho_{\alpha,min}^2 L^3 \frac{\rho_{\alpha,max}^3}{{\rho_{\alpha,min}}^3}\frac{1}{(1-CY^{1/17})} \\ - \epsilon C_M - 8\pi Na \sup_{\mathbf{r}\notin\Lambda_M} \rho_{GP}(\mathbf{r}).\end{aligned} \tag{6.30}$$

Now

$$4\pi Na \sum_{\alpha\subset\Lambda_M} \rho_{\alpha,min}^2 L^3 \leq 4\pi Na \int |\rho_{GP}|^2 \tag{6.31}$$

ρ^{GP} being differentiable and strictly positive and all the cells being included in the fixed cube Λ_M, there exist constants $C_3 < \infty$ and $C_4 > 0$ such that

$$\rho_{\alpha,max} - \rho_{\alpha,min} \leq C_3 L, \quad \rho_{\alpha,min} \geq C_4 \tag{6.32}$$

Remembering that we have chosen $L \sim N^{-\frac{1}{10}}$ and, consequently, $Y \sim N^{-\frac{17}{10}}$, one has for large N

$$\frac{\rho_{\alpha,max}^3}{\rho_{\alpha,min}^3}\frac{1}{(1-CY^{1/17})} \leq 1 + cost\cdot N^{-1/10} \tag{6.33}$$

Finally we obtain from (6.13)

$$\begin{aligned}\frac{E(\rho_N)}{N} - E(\rho_{GP}) \geq 4\pi Na \int |\rho_{GP}|^2 \\ - 4\pi Na \int |\rho_{GP}|^2(1 + const\cdot N^{-1/10}) - N^{-1/10}C_M - 8\pi Na \sup_{\mathbf{r}\notin\Lambda_M} \rho_{GP}(\mathbf{r})\end{aligned} \tag{6.34}$$

Taking $N \uparrow \infty$ and then $M \uparrow \infty$ one obtains the result. In fact the last term is arbitrarily small for M large since ρ_{GP} decreases faster than exponentially at infinity ([29]). □

Proof. (**Energy Localization Theorem**)(see [31] , Lemma 7.3, p.66 or [30] for a sketch of the proof) It is sufficient to show that when $N \uparrow \infty$

$$\int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2 \cdots d\mathbf{r}_N \int_{F_N^c(\mathbf{r}_2,\ldots,\mathbf{r}_N)} (\frac{\nabla_1 F}{F})^2 \rho_N d\mathbf{r}_1 + \int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2 \cdots d\mathbf{r}_N \int \rho_N [\frac{1}{2}\sum_{k\geq 2} v(|\mathbf{r}-\mathbf{r}_k|) - 8\pi N a \rho_{GP}] \geq -4\pi N a \int |\rho_{GP}|^2 d\mathbf{r} - o(1). \tag{6.35}$$

This implies the thesis because (6.35) can be written as

$$\int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2 \cdots d\mathbf{r}_N \int (\frac{\nabla_1 F}{F})^2 \rho_N d\mathbf{r}_1 + \int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2 \cdots d\mathbf{r}_N \int \rho_N [\frac{1}{2}\sum_{k\geq 2} v(|\mathbf{r}-\mathbf{r}_k|) - 8\pi N a \rho_{GP}] - \int_{\mathbb{R}^{3(N-1)}} d\mathbf{r}_2 \cdots d\mathbf{r}_N \int_{F^N(\mathbf{r}_2,\ldots,\mathbf{r}_N)} (\frac{\nabla_1 F}{F})^2 \rho_N d\mathbf{r}_1 \geq -4\pi N a \int |\rho_{GP}|^2 d\mathbf{r} - o(1) \tag{6.36}$$

and from (3.4),(3.5) and (3.6) in the *Energy Theorem* with V particularized to be equal to $8\pi N a \rho_{GP}$ in (3.5) we obtain the thesis. Therefore one has to prove (6.35).
Using the fact that F is *symmetric* in the particle coordinates, one can see that (6.35) is finally equivalent to

$$\frac{Q_\delta(F)}{N} \geq -4\pi N a \int |\phi_{GP}|^4 d\mathbf{r} - o(1) \tag{6.37}$$

where

$$Q_\delta = \sum_{i=1}^N \int_{\Gamma_i^c} |\nabla_i F|^2 \prod_{k=1}^N \rho_{GP}(\mathbf{r}_k) d\mathbf{r}_k + \sum_{1\leq i\leq j\leq N} \int v(|\mathbf{r}_i - \mathbf{r}_j|)|F|^2 \prod_{k=1}^N \rho_{GP}(\mathbf{r}_k) d\mathbf{r}_k \tag{6.38}$$

$$-8\pi N a \sum_{i=1}^N \int \rho_{GP}(\mathbf{r}_i)|F|^2 \prod_{k=1}^N \rho_{GP}(\mathbf{r}_k) d\mathbf{r}_k \tag{6.39}$$

with

$$\Gamma_i^c = \{(\mathbf{r}_1, ..., \mathbf{r}_N) \in \mathbb{R}^{3N} | \min_{k\neq i} |\mathbf{r}_i - \mathbf{r}_k| \leq R'\} \tag{6.40}$$

where $R' = N^{-\frac{1}{3}-\delta}$. Note that Γ_i^c is now a subset of $\mathbb{R}^{3N}$ and not of $\mathbb{R}^3$ like F_N .

We now observe that $Q_\delta(F)$ is essentially the same as $Q(F)$ in the proof of the *Energy Theorem*, the only difference being in the integration domain of the kinetic energy term. Applying the same scheme used for minimizing $Q(F)$, we only need to add the two following remarks

1) Since from (6.9) $\frac{L}{a} \sim Y_\alpha^{-\beta}$ then

$$R \sim LY_\alpha^{1/17} \sim aY_\alpha^{-\beta}Y_\alpha^{1/17} \sim aY_\alpha^{-5/17}$$

having used that $\beta = \frac{6}{17}$. Finally $R \sim N^{-7/17}$.

2) Since the kinetic energy of particle i is now restricted to the subset of $\mathbb{R}^{3N}$ in which $\min_{k\neq i} |\mathbf{r}_i - \mathbf{r}_k| \leq N^{-1/3-\delta}$, in order to apply correctly the *Smoothing Lemma* one must impose that $R \leq N^{-1/3-\delta}$ that is $N^{-7/17} < N^{-1/3-\delta}$ i.e. $\delta \leq 4/51$. Therefore the part of the kinetic energy we have in $Q_\delta(F)$ (according with the hypothesis in *Energy Localization Theorem*) is sufficient to establish the estimate (6.20). The remaining part of the kinetic energy, which is ϵ times the total kinetic energy, is of order $N^{-\frac{2}{17}}$ since $\epsilon = Y_\alpha^{\frac{1}{17}}$ and $Y_\alpha \sim N^{-2}$. Being the total kinetic energy asymptotically finite (see (3.4)), this last part goes to zero when $N \uparrow \infty$.

As in the proof of the *Energy Theorem*, we finally obtain

$$\frac{Q_\delta(F)}{N} \geq -4\pi Na \int (\rho_{GP})^2[1 + const \cdot N^{-1/10}] - Y^{1/17}C_M - 8\pi aN \sup_{\mathbf{r}\notin\Lambda_M} \rho_{GP}(\mathbf{r}) \tag{6.41}$$

Taking $N \uparrow \infty$ and then $M \uparrow \infty$ one obtains the result. □

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