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## ► To cite this version:

Gonca Aki, Jean Dolbeault, Christof Sparber. Thermal effects in gravitational Hartree systems. Annales Henri Poincaré, 2011, 12, pp.1055-1079. hal-00512641

**HAL Id: hal-00512641**

**<https://hal.science/hal-00512641>**

Submitted on 31 Aug 2010

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# THERMAL EFFECTS IN GRAVITATIONAL HARTREE SYSTEMS

GONCA L. AKI, JEAN DOLBEAULT, AND CHRISTOF SPARBER

**ABSTRACT.** We consider the non-relativistic Hartree model in the gravitational case, i.e. with attractive Coulomb-Newton interaction. For a given mass  $M > 0$ , we construct stationary states with non-zero temperature  $T$  by minimizing the corresponding free energy functional. It is proved that minimizers exist if and only if the temperature of the system is below a certain threshold  $T^* > 0$  (possibly infinite), which itself depends on the specific choice of the entropy functional. We also investigate whether the corresponding minimizers are mixed or pure quantum states and characterize a critical temperature  $T_c \in (0, T^*)$  above which mixed states appear.

## 1. INTRODUCTION

In this paper we investigate the *non-relativistic gravitational Hartree system with temperature*. This model can be seen as a mean-field description of a system of self-gravitating quantum particles. It is used in astrophysics to describe so-called *Boson stars*. In the present work, we are particularly interested in *thermal effects*, i.e. (qualitative) differences to the zero temperature case.

A physical state of the system will be represented by a density matrix operator  $\rho \in \mathfrak{S}_1(L^2(\mathbb{R}^3))$ , i.e. a positive self-adjoint trace class operator acting on  $L^2(\mathbb{R}^3; \mathbb{C})$ . Such an operator  $\rho$  can be decomposed as

$$(1.1) \quad \rho = \sum_{j \in \mathbb{N}} \lambda_j |\psi_j\rangle\langle\psi_j|$$

with an associated sequence of eigenvalues  $(\lambda_j)_{j \in \mathbb{N}} \in \ell^1$ ,  $\lambda_j \geq 0$ , usually called *occupation numbers*, and a corresponding sequence of eigenfunction  $(\psi_j)_{j \in \mathbb{N}}$ , forming a complete orthonormal basis of  $L^2(\mathbb{R}^3)$ , cf. [33]. By evaluating the kernel  $\rho(x, y)$  on its diagonal, we obtain the corresponding particle density

$$n_\rho(x) = \sum_{j \in \mathbb{N}} \lambda_j |\psi_j(x)|^2 \in L^1_+(\mathbb{R}^3) .$$

In the following we shall assume that

$$(1.2) \quad \int_{\mathbb{R}^3} n_\rho(x) \, dx = M ,$$

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*Date:* August 31, 2010.

*2010 Mathematics Subject Classification.* 35Q40, 47G20, 49J40, 82B10, 85A15.

*Key words and phrases.* Gravitation, Hartree energy, entropy, ground states, free energy, Casimir functional, pure states, mixed states.

This publication has been supported by Award No. KUK-I1-007-43 of the King Abdullah University of Science and Technology (KAUST). J. Dolbeault and C. Sparber have been supported, respectively, by the ANR-08-BLAN-0333-01 project CBDif-Fr and by the University research fellowship of the Royal Society. G.L. Aki acknowledges the support of the FWF, grant no. W 800-N05 and funding by WWTF project (MA45).

for a given total mass  $M > 0$ . We assume that the particles interact solely via gravitational forces. The corresponding *Hartree energy* of the system is then given by

$$\mathcal{E}_H[\rho] := \mathcal{E}_{\text{kin}}[\rho] - \mathcal{E}_{\text{pot}}[\rho] = \text{tr}(-\Delta \rho) - \frac{1}{2} \text{tr}(V_\rho \rho),$$

where  $V_\rho$  denotes the *self-consistent potential*

$$V_\rho = n_\rho * \frac{1}{|\cdot|}$$

and ‘ $*$ ’ is the usual convolution w.r.t.  $x \in \mathbb{R}^3$ . Using the decomposition (1.1) for  $\rho$ , the Hartree energy can be rewritten as

$$\mathcal{E}_H[\rho] = \sum_{j \in \mathbb{N}} \lambda_j \int_{\mathbb{R}^3} |\nabla \psi_j(x)|^2 dx - \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{n_\rho(x) n_\rho(y)}{|x - y|} dx dy.$$

To take into account thermal effects, we consider the associated *free energy functional*

$$(1.3) \quad \mathcal{F}_T[\rho] := \mathcal{E}_H[\rho] - T \mathcal{S}[\rho]$$

where  $T \geq 0$  denotes the temperature and  $\mathcal{S}[\rho]$  is the *entropy functional*

$$\mathcal{S}[\rho] := -\text{tr} \beta(\rho).$$

The *entropy generating function*  $\beta$  is assumed to be convex, of class  $C^1$  and will satisfy some additional properties to be prescribed later on. The purpose of this paper is to investigate the existence of *minimizers* for  $\mathcal{F}_T$  with fixed mass  $M > 0$  and temperature  $T \geq 0$  and study their qualitative properties. These minimizers, often called *ground states*, can be interpreted as stationary states for the time-dependent system

$$(1.4) \quad i \frac{d}{dt} \rho(t) = [H_{\rho(t)}, \rho(t)], \quad \rho(0) = \rho_{\text{in}}.$$

Here  $[A, B] = AB - BA$  denotes the usual commutator and  $H_\rho$  is the mean-field *Hamiltonian operator*

$$(1.5) \quad H_\rho := -\Delta - n_\rho * \frac{1}{|\cdot|}.$$

Using again the decomposition (1.1), this can equivalently be rewritten as a system of (at most) countably many Schrödinger equations coupled through the mean field potential  $V_\rho$ :

$$(1.6) \quad \begin{cases} i \partial_t \psi_j + \Delta \psi_j + V(t, x) \psi_j = 0, & j \in \mathbb{N}, \\ -\Delta V_\rho = 4\pi \sum_{j \in \mathbb{N}} \lambda_j |\psi_j(t, x)|^2. \end{cases}$$

This system is a generalization of the gravitational Hartree equation (also known as the *Schrödinger-Newton model*, see [5]) to the case of mixed states. Notice that it reduces to a finite system as soon as only a finite number of  $\lambda_j$  are non-zero. In such a case,  $\rho$  is a finite rank operator.

Establishing the existence of stationary solutions to nonlinear Schrödinger models by means of variational methods is a classical idea, cf. for instance [15]. A particular advantage of such an approach is that in most cases one can directly deduce *orbital stability* of the stationary solution w.r.t. the dynamics of (1.4) or, equivalently, (1.6). In the case of *repulsive* self-consistent interactions, describing e.g. electrons, this has been successfully carried out in [6, 7, 8, 24]. In addition, existence of stationary solutions in the repulsive case has been obtained in [23, 25, 26, 27] using convexity properties of the corresponding energy functional.

In sharp contrast to the repulsive case, the gravitational Hartree system of stellar dynamics, does *not* admit a convex energy and thus a more detailed study of minimizing sequences is required. To this end, we first note that at zero temperature, i.e.  $T = 0$ , the free energy  $\mathcal{F}_T[\rho]$  reduces to the gravitational Hartree energy  $\mathcal{E}_H[\rho]$ . For this model, existence of the corresponding zero temperature ground states has been studied in [14, 17, 19] and, more recently, in [5]. Most of these works rely on the so-called *concentration-compactness method* introduced by Lions in [18]. According to [14], it is known that for  $T = 0$  the minimum of the Hartree energy is uniquely achieved by an appropriately normalized *pure state*, i.e. a rank one density matrix  $\rho_0 = M |\psi_0\rangle\langle\psi_0|$ . The concentration-compactness method has later been adapted to the setting of density matrices, see for instance [13] for a recent paper written this framework, in which the authors study a *semi-relativistic* model of Hartree-Fock type at zero temperature.

**Remark 1.1.** In the classical kinetic theory of self-gravitating systems, a variational approach based on the so-called *Casimir functionals* has been repeatedly used to prove existence and orbital stability of stationary states of relativistic and non-relativistic Vlasov-Poisson models: see for instance [34, 35, 36, 28, 29, 32, 9, 30, 31]. These functionals can be regarded as the classical counterpart of  $\mathcal{F}_T[\rho]$  and such an analogy between classical and quantum mechanics has already been used in [24, 7, 8, 6].

In view of the quoted results, the purpose of this paper can be summarized as follows: First, we shall prove the existence of minimizers for  $\mathcal{F}_T$ , extending the results of [14, 17, 19, 5] to the case of non-zero temperature. As we shall see, a *threshold in temperature* arises due to the competition between the Hartree energy and the entropy term and we find that minimizers of  $\mathcal{F}_T$  exist only *below a certain maximal temperature*  $T^* > 0$ , which depends on the specific form of the entropy generating function  $\beta$ . One should note that, by using the scaling properties of the system, the notion of a maximal temperature for a given mass  $M$  can be rephrased into a corresponding threshold for the mass at a given, fixed temperature  $T$ . Such a critical mass, however, has to be clearly distinguished from the well-known *Chandrasekhar mass* threshold in semi-relativistic models, cf. [16, 11, 13]. Moreover, depending on the choice of  $\beta$ , it could happen that  $T^* = +\infty$ , in which case minimizers of  $\mathcal{F}_T$  would exist even if the temperature is taken arbitrarily large. In a second step, we shall also study the qualitative properties of the ground states with respect to the temperature  $T \in [0, T^*)$ . In particular, we will prove that there exists a certain *critical temperature*  $T_c > 0$ , above which minimizers correspond to *mixed quantum states*, i.e. density matrix operators with rank higher than one. If  $T < T_c$ , minimizers are pure states, as in the zero temperature model.

In order to make these statements mathematically precise, we introduce

$$\mathfrak{H} := \left\{ \rho : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3) : \rho \geq 0, \rho \in \mathfrak{S}_1, \sqrt{-\Delta} \rho \sqrt{-\Delta} \in \mathfrak{S}_1 \right\}$$

and consider the norm

$$\|\rho\|_{\mathfrak{H}} := \text{tr } \rho + \text{tr} \left( \sqrt{-\Delta} \rho \sqrt{-\Delta} \right).$$

The set  $\mathfrak{H}$  can be interpreted as the cone of nonnegative density matrix operators with finite energy. Using the decomposition (1.1), if  $\rho \in \mathfrak{H}$ , we obtain that  $\psi_j \in H^1(\mathbb{R}^3)$  for all  $j \in \mathbb{N}$  such that  $\lambda_j > 0$ . Taking into account the mass constraint (1.2) we define the set of physical states by

$$\mathfrak{H}_M := \{ \rho \in \mathfrak{H} : \text{tr } \rho = M \}.$$

We denote the infimum of the free energy functional  $\mathcal{F}_T$ , defined in (1.3), by

$$(1.7) \quad i_{M,T} = \inf_{\rho \in \mathfrak{H}_M} \mathcal{F}_T[\rho] .$$

The set of minimizers will be denoted by  $\mathfrak{M}_M \subset \mathfrak{H}_M$ . As we shall see in the next section,  $i_{M,T} < 0$  if  $\mathfrak{M}_M \neq \emptyset$ . This however can be guaranteed only below a certain maximal temperature  $T^* = T^*(M)$  given by

$$(1.8) \quad T^*(M) := \sup\{T > 0 : i_{M,T} < 0\} .$$

This maximal temperature  $T^*$  will depend on the choice of the entropy generating function  $\beta$  for which we impose the following assumptions:

( $\beta 1$ )  $\beta$  is strictly convex and of class  $C^1$  on  $[0, \infty)$ ,

( $\beta 2$ )  $\beta \geq 0$  on  $[0, 1]$  and  $\beta(0) = \beta'(0) = 0$ ,

( $\beta 3$ )  $\sup_{m \in (0, \infty)} \frac{m \beta'(m)}{\beta(m)} \leq 3$ .

A typical example for the function  $\beta$  reads

$$\beta(s) = s^p, \quad p \in (1, 3] .$$

Such a power law nonlinearity is of common use in the classical kinetic theory of self-gravitating systems known as *polytropic gases*. One of the main features of such models is to give rise to orbitally stable stationary states with *compact support*, cf. [10, 29, 30, 34, 35, 36], clearly a desirable feature when modeling stars. We shall prove in Section 6, that  $T^*$  is *finite* if  $p$  is not too large. The limiting case as  $p$  approaches 1 corresponds to  $\beta(s) = s \ln s$  but in that case the free energy functional is *not* bounded from below, see [21] for a discussion in the Coulomb repulsive case, which can easily be adapted to our setting.

Up to now, we have made no distinction between *pure states*, corresponding density matrix operators with rank one, and *mixed states*, corresponding to operators with finite or infinite rank. In [14] Lieb has proved that for  $T = 0$  minimizers are pure states. As we shall see, this is also the case when  $T$  is positive but small and as a consequence we have:  $i_{M,T} = i_{M,0} + T \beta(M)$ . Let us define

$$(1.9) \quad T_c(M) := \max\{T > 0 : i_{M,T} = i_{M,0} + \tau \beta(M) \ \forall \tau \in (0, T]\} .$$

With these definitions in hand, we are now in the position to state our main result.

**Theorem 1.1.** *Let  $M > 0$  and assume that ( $\beta 1$ )–( $\beta 3$ ) hold. Then, the maximal temperature  $T^*$  defined in (1.8) is positive, possibly infinite, and the following properties hold:*

- (i) *For all  $T < T^*$ , there exists a density operator  $\rho \in \mathfrak{H}_M$  such that  $\mathcal{F}_T[\rho] = i_{M,T}$ . Moreover  $\rho$  solves the self-consistent equation*

$$\rho = (\beta')^{-1}((\mu - H_\rho)/T)$$

*where  $H_\rho$  is the mean-field Hamiltonian defined in (1.5) and  $\mu < 0$  denotes the Lagrange multiplier associated to the mass constraint.*

- (ii) *The set of all minimizers  $\mathfrak{M}_M \subset \mathfrak{H}_M$  is orbitally stable under the dynamics of (1.4).*
- (iii) *The critical temperature  $T_c$  defined in (1.9) is finite and a minimizer  $\rho \in \mathfrak{M}_M$  is a pure state if and only if  $T \in [0, T_c]$ .*
- (iv) *If, in addition,  $\beta(s) = s^p$  with  $p \in (1, 7/5)$ , then  $T^* < +\infty$ .*

The proof of this theorem will be a consequence of several more detailed results. We shall mostly rely on the concentration-compactness method, adapted to the framework of trace class operators. Our approach is therefore similar to the one of [6] and [13], with differences due, respectively, to the sign of the interaction potential and to non-zero temperature effects. Uniqueness of minimizers (up to translations and rotations) is an open question for  $T > T_c$ . For  $T \in [0, T_c]$ , the problem is reduced to the pure state case, for which uniqueness has been proved in [14] (also see [12]).

This paper is organized as follows: In Section 2 we collect several basic properties of the free energy. In particular we establish the existence of a maximal temperature  $T^* > 0$  and derive the self-consistent equation for  $\rho \in \mathfrak{H}_M$ . In Section 3, we derive an important a priori inequality for minimizers, the so-called *binding inequality*, which is henceforth used in proving the existence of minimizers in Section 4. Having done that, we shall prove in Section 5 that minimizers are mixed states for  $T > T_c$ , and we shall also characterize  $T_c$  in terms of the eigenvalue problem associated to the case  $T = 0$ . In Section 6, we shall prove that  $T^*$  is indeed finite in the polytropic case, provided  $p < 7/5$  and furthermore establish some qualitative properties of the minimizers as  $T \rightarrow T^* < +\infty$ . Finally, Section 7 is devoted to some remarks on the sign of the Lagrange multiplier associated to the mass constraint and related open questions.

## 2. BASIC PROPERTIES OF THE FREE ENERGY

**2.1. Boundedness from below and splitting property.** As a preliminary step, we observe that the functional  $\mathcal{F}_T$  introduced in (1.3) is well defined and  $i_{M,T} > -\infty$ .

**Lemma 2.1.** *Assume that  $(\beta 1)$ – $(\beta 2)$  hold. The free energy  $\mathcal{F}_T$  is well-defined on  $\mathfrak{H}_M$  and  $i_{M,T}$  is bounded from below. If  $\mathcal{F}_T[\rho]$  is finite, then  $\sqrt{n_\rho}$  is bounded in  $H^1(\mathbb{R}^3)$ .*

*Proof.* In order to establish a bound from below, we shall first show that the potential energy  $\mathcal{E}_{\text{pot}}[\rho]$  can be bounded in terms of the kinetic energy. To this end, note that for every  $\rho \in \mathfrak{H}$  we have

$$\mathcal{E}_{\text{pot}}[\rho] \leq C \|n_\rho\|_{L^1}^{3/2} \|n_\rho\|_{L^3}^{1/2}$$

by the Hardy-Littlewood-Sobolev inequality. Next, by Sobolev's embedding, we know that  $\|n_\rho\|_{L^3}$  is controlled by  $\|\nabla \sqrt{n_\rho}\|_{L^2}^2$  which, using the decomposition (1.1), is bounded by  $\text{tr}(-\Delta \rho)$ . Hence we can conclude that

$$(2.1) \quad \mathcal{E}_{\text{pot}}[\rho] \leq C \|n_\rho\|_{L^1}^{3/2} \text{tr}(-\Delta \rho)^{1/2}$$

for some generic positive constant  $C$ . By conservation of mass, the free energy is therefore bounded from below on  $\mathfrak{H}_M$  according to

$$\mathcal{F}_T[\rho] \geq \text{tr}(-\Delta \rho) - C M^{3/2} \text{tr}(-\Delta \rho)^{1/2} \geq -\frac{1}{4} C^2 M^3$$

uniformly w.r.t.  $\rho \in \mathcal{H}_M$ , thus establishing a lower bound on  $i_{M,T}$ . For the entropy term  $\mathcal{S}[\rho] = -\text{tr} \beta(\rho)$  we observe that, since  $\beta$  is convex and  $\beta(0) = 0$ , it holds  $0 \leq \beta(\rho) \leq \beta(M) \rho$  for all  $\rho \in \mathfrak{H}$  and  $\beta(\rho) \in \mathfrak{S}_1$ , provided  $\rho \in \mathfrak{S}_1$ . Hence, all quantities involved in the definition of  $\mathcal{F}_T$  are well-defined and bounded on  $\mathfrak{H}_M$ .  $\square$

Throughout this work, we shall use smooth *cut-off functions* defined as follows. Let  $\chi$  be a fixed smooth function on  $\mathbb{R}^3$  with values in  $[0, 1]$  such that, for any  $x \in \mathbb{R}^3$ ,  $\chi(x) = 1$  if

$|x| < 1$  and  $\chi(x) = 0$  if  $|x| \geq 2$ . For any  $R > 0$ , we define  $\chi_R$  and  $\xi_R$  by

$$(2.2) \quad \chi_R(x) = \chi(x/R) \quad \text{and} \quad \xi_R(x) = \sqrt{1 - \chi(x/R)^2} \quad \forall x \in \mathbb{R}^3.$$

The motivation for introducing such cut-off functions is that, for any  $u \in H^1(\mathbb{R}^3)$  and any potential  $V$ , we have the identities

$$\begin{aligned} \int_{\mathbb{R}^3} |u|^2 dx &= \int_{\mathbb{R}^3} |\chi_R u|^2 dx + \int_{\mathbb{R}^3} |\xi_R u|^2 dx \\ \text{and} \quad \int_{\mathbb{R}^3} V |u|^2 dx &= \int_{\mathbb{R}^3} V |\chi_R u|^2 dx + \int_{\mathbb{R}^3} V |\xi_R u|^2 dx, \end{aligned}$$

and the IMS truncation identity

$$(2.3) \quad \int_{\mathbb{R}^3} |\nabla(\chi_R u)|^2 dx + \int_{\mathbb{R}^3} |\nabla(\xi_R u)|^2 dx = \int_{\mathbb{R}^3} |\nabla u|^2 dx - \int_{\mathbb{R}^3} |u|^2 \underbrace{\nabla \cdot (\nabla \chi_R + \nabla \xi_R)}_{=O(R^{-2}) \text{ as } R \rightarrow \infty} dx.$$

A first application of this truncation method is given by the following splitting lemma.

**Lemma 2.2.** *For  $\rho \in \mathfrak{H}_M$ , we define  $\rho_R^{(1)} = \chi_R \rho \chi_R$  and  $\rho_R^{(2)} = \xi_R \rho \xi_R$ . Then it holds:*

$$\mathcal{S}[\rho_R^{(1)}] + \mathcal{S}[\rho_R^{(2)}] \geq \mathcal{S}[\rho] \quad \text{and} \quad \mathcal{E}_{\text{kin}}[\rho_R^{(1)}] + \mathcal{E}_{\text{kin}}[\rho_R^{(2)}] \leq \mathcal{E}_{\text{kin}}[\rho] + O(R^{-2}) \quad \text{as } R \rightarrow +\infty.$$

*Proof.* The assertion for  $\mathcal{E}_{\text{kin}}[\rho]$  is a straightforward consequence of (2.3), namely

$$\text{tr}(-\Delta \rho_R^{(1)}) + \text{tr}(-\Delta \rho_R^{(2)}) = \text{tr}(-\Delta \rho) + O(R^{-2}) \quad \text{as } R \rightarrow +\infty.$$

For the entropy term, we can use the *Brown-Kosaki inequality* (cf. [2]) as in [6, Lemma 3.4] to obtain

$$\text{tr} \beta(\rho_R^{(1)}) + \text{tr} \beta(\rho_R^{(2)}) \leq \text{tr} \beta(\rho).$$

□

**2.2. Sub-additivity and maximal temperature.** In order to proceed further, we need to study the dependence of  $i_{M,T}$  with respect to  $M$  and  $T$  and prove that the maximal temperature  $T^*$  as defined in (1.8) is in fact positive. To this end, we rely on the translation invariance of the model. For a given  $y \in \mathbb{R}^3$ , denote by  $\tau_y : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$  the translation operator given by

$$(\tau_y f) = f(\cdot - y) \quad \forall f \in L^2(\mathbb{R}^3).$$

**Proposition 2.3.** *Let  $i_{M,T}$  be given by (1.7) and assume that  $(\beta 1)$ – $(\beta 2)$  hold. Then the following properties hold:*

- (i) *As a function of  $M$ ,  $i_{M,T}$  is non-positive and sub-additive: for any  $M > 0$ ,  $m \in (0, M)$  and  $T > 0$ , we have*

$$i_{M,T} \leq i_{M-m,T} + i_{m,T} \leq 0.$$

- (ii) *The function  $i_{M,T}$  is a non-increasing function of  $M$  and a non-decreasing function of  $T$ . For any  $T > 0$ , we have  $i_{M,T} < 0$  if and only if  $T < T^*$ .*
- (iii) *For any  $M > 0$ ,  $T^*(M) > 0$  is positive, possibly infinite. As a function of  $M$  it is increasing and satisfies*

$$T^*(M) \geq \max_{0 \leq m \leq M} \frac{m^3}{\beta(m)} |i_{1,0}|.$$

*As a consequence,  $T^* > 0$  and  $T^*(M) = +\infty$  for any  $M > 0$  if  $\lim_{s \rightarrow 0+} \beta(s)/s^3 = 0$ .*

*Proof.* We start with the proof of the sub-additivity inequality. Consider two states  $\rho \in \mathfrak{H}_{M-m}$  and  $\sigma \in \mathfrak{H}_m$ , such that  $\mathcal{F}_T[\rho] \leq i_{M-m,T} + \varepsilon$  and  $\mathcal{F}_T[\sigma] \leq i_{m,T} + \varepsilon$ . By density of finite rank operators in  $\mathfrak{H}$  and of smooth compactly supported functions in  $L^2$ , we can assume that

$$\rho = \sum_{j=1}^J \lambda_j |\psi_j\rangle\langle\psi_j| ,$$

with smooth eigenfunctions  $(\psi_j)_{j=1}^J$  having compact support in a ball  $B(0, R) \subset \mathbb{R}^3$ , for some  $J \in \mathbb{N}$ . After approximating  $\sigma$  analogously, we define  $\sigma_{Re} := \tau_{3Re}^* \sigma \tau_{3Re}$ , where  $e \in \mathbb{S}^2 \subset \mathbb{R}^3$  is a fixed unit vector and  $\tau$  is the translation operator defined above. Note that we have  $\rho \sigma_{Re} = \sigma_{Re} \rho = 0$ , hence  $\rho + \sigma_{Re} \in \mathfrak{H}_M$  and  $\text{tr} \beta(\rho + \sigma_{Re}) = \text{tr} \beta(\rho) + \text{tr} \beta(\sigma_{Re})$ . Thus we have

$$i_{M,T} \leq \mathcal{F}_T[\rho + \sigma_{Re}] = \mathcal{F}_T[\rho] + \mathcal{F}_T[\sigma] + O(1/R) \leq i_{M-m,T} + i_{m,T} + 2\varepsilon ,$$

where the  $O(1/R)$  term has in fact negative sign so that we can simply drop it. Taking the limit  $\varepsilon \rightarrow 0$  yields the desired inequality.

Next, consider a minimizer  $\rho$  of  $\mathcal{E}_H$  subject to  $\text{tr} \rho = M$ . It is given by an appropriate rescaling of the pure state obtained in [14]. For an arbitrary  $\lambda \in (0, \infty)$ , let  $(U_\lambda f)(x) := \lambda^{3/2} f(\lambda x)$  and observe that  $\rho_\lambda := U_\lambda^* \rho U_\lambda \in \mathfrak{H}_M$ . As a function of  $\lambda$ , the Hartree energy  $\mathcal{E}_H[\rho_\lambda] = \lambda^2 \mathcal{E}_{\text{kin}}[\rho] - \lambda \mathcal{E}_{\text{pot}}[\rho]$  has a minimum for some  $\lambda > 0$ . Computing  $\frac{d}{d\lambda} \mathcal{E}_H[\rho_\lambda] = 0$ , we infer that  $\lambda = \mathcal{E}_{\text{pot}}[\rho] / (2 \mathcal{E}_{\text{kin}}[\rho])$  and moreover

$$i_{M,0} \equiv \mathcal{E}_H[\rho] = -\frac{1}{4} \frac{(\mathcal{E}_{\text{pot}}[\rho])^2}{\mathcal{E}_{\text{kin}}[\rho]} .$$

As a consequence, we have  $i_{M,0} = M^3 i_{1,0}$  and

$$(2.4) \quad \mathcal{F}_T[\rho] = i_{M,0} + T \beta(M) = \beta(M) \left( T - \frac{M^3}{\beta(M)} |i_{1,0}| \right) \geq i_{M,T} ,$$

thus proving that  $i_{M,T} < 0$  for  $T$  small enough.

Since  $\beta$  is non-negative function on  $[0, \infty)$ , the map  $T \mapsto \mathcal{F}_T[\rho]$  is increasing. By taking the infimum over all admissible  $\rho \in \mathfrak{H}_M$ , we infer that  $T \mapsto i_{M,T}$  is non-decreasing. The function  $M \mapsto i_{M,T}$  is non-increasing as a consequence of the sub-additivity property. As a consequence,  $T^*(M)$  is a non-decreasing function of  $M$ , such that

$$T^*(M) \geq \lim_{M \rightarrow 0_+} T^*(M) .$$

By the sub-additivity inequality and (2.4), we obtain

$$i_{M,T} \leq n i_{M/n,T} \leq n \beta\left(\frac{M}{n}\right) T - \frac{M^3}{n^2} |i_{1,0}| = n \beta\left(\frac{M}{n}\right) \left( T - \frac{M^3}{n^3 \beta\left(\frac{M}{n}\right)} |i_{1,0}| \right)$$

for any  $n \in \mathbb{N}^*$ . Since  $\lim_{s \rightarrow 0_+} \beta(s)/s = 0$ , we find that  $i_{M,T} \leq 0$  by passing to the limit as  $n \rightarrow \infty$ . In the particular case  $\lim_{s \rightarrow 0_+} \beta(s)/s^3 = 0$ , we conclude that  $T^*(M) = +\infty$  for any  $M > 0$ . Similarly, using again the sub-additivity inequality and (2.4), we infer

$$i_{M,T} \leq i_{m,T} \leq \beta(m) \left( T - \frac{m^3}{\beta(m)} |i_{1,0}| \right) \quad \forall m \in (0, M] ,$$

which provides the lower bound on  $T^*(M)$  in assertion (iii). By definition of  $T^*(M)$ , we also know that  $i_{M,T}$  is negative for any  $T < T^*(M)$ . From the monotonicity of  $T \mapsto i_{M,T}$ , we obtain



that  $i_{M,T} = 0$  if  $T > T^*$  and  $T^* < \infty$ . Because of the estimate  $i_{M,T} \leq i_{M,T_0} + (T - T_0) \beta(M)$  for any  $T > T_0$ , we also find that  $i_{M,T^*} = 0$  if  $T^* < \infty$ .  $\square$

**2.3. Euler-Lagrange equations and Lagrange multipliers.** As in [8, 6], we obtain the following characterization of  $\rho \in \mathfrak{M}_M$ .

**Proposition 2.4.** *Let  $M > 0$ ,  $T \in (0, T^*(M)]$  and assume that  $(\beta 1)$ – $(\beta 2)$  hold. Consider a density matrix operator  $\rho \in \mathfrak{H}_M$  which minimizes  $\mathcal{F}_T$ . Then  $\rho$  is such that*

$$(2.5) \quad \text{tr}(V_\rho \rho) = 4 \text{tr}(-\Delta \rho)$$

and satisfies the self-consistent equation

$$(2.6) \quad \rho = (\beta')^{-1}((\mu - H_\rho)/T),$$

where  $H_\rho$  is the mean-field Hamiltonian defined in (1.5) and  $\mu \leq 0$  denotes the Lagrange multiplier associated to the mass constraint  $\text{tr} \rho = M$ . Explicitly,  $\mu$  is given by

$$(2.7) \quad \mu = \frac{1}{M} \text{tr}((H_\rho + T \beta'(\rho)) \rho).$$

*Proof.* Let  $\rho \in \mathfrak{M}_M$  be a minimizer of  $\mathcal{F}_T$ . Consider the decomposition given by (1.1). If we denote by  $\rho_\lambda$  the density operator in  $\mathfrak{H}_M$  given by

$$\rho_\lambda = \lambda^3 \sum_{j \in \mathbb{N}} \lambda_j |\psi_j(\lambda \cdot)\rangle \langle \psi_j(\lambda \cdot)|,$$

then, as in the proof of Proposition 2.3, we find that  $\mathcal{E}_H[\rho_\lambda] = \lambda^2 \mathcal{E}_{\text{kin}}[\rho] - \lambda \mathcal{E}_{\text{pot}}[\rho]$  while  $\mathcal{S}[\rho_\lambda] = \mathcal{S}[\rho]$  for any  $\lambda > 0$ . Hence the condition  $\frac{d}{d\lambda} \mathcal{E}_H[\rho_\lambda]|_{\lambda=1} = 0$  exactly amounts to  $\mathcal{E}_{\text{pot}}[\rho] = 2 \mathcal{E}_{\text{kin}}[\rho]$ . Next, let  $\sigma \in \mathfrak{H}_M$ . Then  $(1-t)\rho + t\sigma \in \mathfrak{H}_M$  and

$$t \mapsto \mathcal{F}_T[(1-t)\rho + t\sigma]$$

has a minimum at  $t = 0$ . Computing its derivative at  $t = 0$  and arguing by contradiction implies that  $\rho$  also solves the linearized problem

$$\inf_{\sigma \in \mathfrak{H}_M} \text{tr}((H_\rho + T \beta'(\rho))(\sigma - \rho)).$$

Computing the corresponding Euler-Lagrange equations shows that the minimizer of this problem is  $\rho = (\beta')^{-1}((\mu - H_\rho)/T)$  where  $\mu$  denotes the Lagrange multiplier associated to the constraint  $\text{tr} \rho = M$ . Since the essential spectrum of  $H_\rho$  is  $[0, \infty)$ , we also get that  $\mu \leq 0$  since  $\rho$  is trace class and  $(\beta')^{-1} > 0$  on  $(0, \infty)$ .  $\square$

Using the decomposition (1.1) we can rewrite the stationary Hartree model in terms of (at most) countably many eigenvalue problems coupled through a nonlinear Poisson equation

$$\begin{cases} \Delta \psi_j + V_\rho \psi_j + \mu_j \psi_j = 0, & j \in \mathbb{N}, \\ -\Delta V_\rho = 4\pi \sum_{j \in \mathbb{N}} \lambda_j |\psi_j|^2, \end{cases}$$

where  $(\mu_j)_{j \in \mathbb{N}} \in \mathbb{R}$  denotes the sequence of the eigenvalues of  $H_\rho$  and  $\langle \psi_j, \psi_k \rangle_{L^2} = \delta_{j,k}$ . The self-consistent equation (2.6) consequently implies the following relation between the occupation numbers  $(\lambda_j)_{j \in \mathbb{N}}$  and the eigenvalues  $(\mu_j)_{j \in \mathbb{N}}$ :

$$(2.8) \quad \lambda_j = (\beta')^{-1}((\mu - \mu_j)/T)_+,$$

where  $s_+ = (s + |s|)/2$  denotes the positive part of  $s$ . Upon reverting the relation (2.8) we obtain  $\mu_j = \mu - T \beta'(\lambda_j)$  for any  $\mu_j \leq \mu$ .

The Lagrange multiplier  $\mu$  is usually referred to as the *chemical potential*. In the existence proof given below, it will be essential, that  $\mu < 0$ . In order to show that this is indeed the case, let  $p(M) := \sup_{m \in (0, M]} \frac{m \beta'(m)}{\beta(m)}$ . If  $\rho \in \mathfrak{H}_M$ , then

$$\mathrm{tr}(\beta'(\rho) \rho) \leq p(M) \mathrm{tr} \beta(\rho) .$$

Notice that if  $(\beta 3)$  holds, then  $p(M) \leq 3$ .

**Lemma 2.5.** *Let  $M > 0$  and  $T < T^*(M)$ . Assume that  $\rho \in \mathfrak{H}_M$  is a minimizer of  $\mathcal{F}_T$  and let  $\mu$  be the corresponding Lagrange multiplier. With the above notations, if  $p(M) \leq 3$ , then  $M \mu \leq p(M) i_{M,T} < 0$ .*

*Proof.* By definition of  $i_{M,T}$  and according to (2.7), we know that

$$\begin{aligned} i_{M,T} &= \mathrm{tr} \left( -\Delta \rho - \frac{1}{2} V_\rho \rho + T \beta(\rho) \right) , \\ M \mu &= \mathrm{tr} \left( -\Delta \rho - V_\rho \rho + T \beta'(\rho) \rho \right) . \end{aligned}$$

Using (2.5), we end up with the identity

$$p(M) i_{M,T} - M \mu = (3 - p(M)) \mathrm{tr}(-\Delta \rho) + T \mathrm{tr} (p(M) \beta(\rho) - \beta'(\rho) \rho) \geq 0 ,$$

which concludes the proof.  $\square$

The negativity of the Lagrange multiplier  $\mu$ , is straightforward in the zero temperature case. In our situation it holds under Assumption  $(\beta 3)$ , but has not been established for instance for  $\beta(s) = s^p$  with  $p > 3$ . In fact, it might even be false in some cases, see Section 7 for more details.

**Corollary 2.6.** *Let  $T > 0$ . Then  $M \mapsto i_{M,T}$  is monotone decreasing as long as  $T < T^*(M)$  and  $p(M) \leq 3$ .*

*Proof.* Let  $\rho \in \mathfrak{H}_M$  be such that  $\mathcal{F}_T[\rho] \leq i_{M,T} + \varepsilon$ , for some  $\varepsilon > 0$  to be chosen. With no restriction, we can assume that  $\mathcal{E}_{\mathrm{pot}}[\rho] = 2 \mathcal{E}_{\mathrm{kin}}[\rho]$  and define  $\mu[\rho] := \frac{d}{d\lambda} \mathcal{F}_T[\lambda \rho]_{|\lambda=1}$ . The same computation as in the proof of Lemma 2.5 shows that

$$p(M) (i_{M,T} + \varepsilon) - M \mu \geq (3 - p(M)) \mathrm{tr}(-\Delta \rho) + T \mathrm{tr} (p(M) \beta(\rho) - \beta'(\rho) \rho) \geq 0 ,$$

since, by assumption,  $p(M) \leq 3$ . This proves that  $M \mu[\rho] < i_{M,T}/2 < 0$  for any  $\varepsilon \in (0, |i_{M,T}|/2)$ , if  $p(M) \leq 3$ . This bound being uniform with respect to  $\rho$ , monotonicity easily follows.  $\square$

**Remark 2.7.** Under the assumptions of Lemma 2.5, we observe that

$$\frac{d}{d\lambda} \mathcal{F}_T[\lambda \rho]_{|\lambda=1} = \mu M < 0 ,$$

provided  $p(M) \leq 3$  and  $\rho \in \mathfrak{H}_M$ , which proves the strict monotonicity of  $M \mapsto i_{M,T}$ . However, at this stage, the existence of a minimizer is not granted and we thus had to argue differently.

### 3. THE BINDING INEQUALITY

In this section we shall strengthen the result of Proposition 2.3 (i) and infer a *strict* sub-additivity property of  $i_{M,T}$ , which is usually called the *binding inequality*; see e.g. [13]. This will appear as a consequence of the following a priori estimate for the spatial density of the minimizers.

**Proposition 3.1.** *Let  $\rho \in \mathfrak{H}_M$  be a minimizer of  $\mathcal{F}_T$ . There exists a positive constant  $C$  such that, for all  $R > 0$  sufficiently large,*

$$\int_{|x|>R} n_\rho(x) \, dx \leq \frac{C}{R^2}.$$

This result is the analog of [13, Lemma 5.2]. For completeness, we shall give the details of the proof, which requires  $\mu < 0$ , in the appendix. The following elementary estimate will be useful in the sequel.

**Lemma 3.2.** *There exists a positive constant  $C$  such that, for any  $\rho \in \mathfrak{H}_M$ ,*

$$\int_{\mathbb{R}^3} \frac{n_\rho(x)}{|x|} \, dx \leq C M^{3/2} (\operatorname{tr}(-\Delta \rho))^{1/2}.$$

*Proof.* Up to a translation, we have to estimate  $\int_{\mathbb{R}^3} |x|^{-1} n_\rho(x) \, dx$  and it is convenient to split the integral into two integrals corresponding to  $|x| \leq R$  and  $|x| > R$ . By Hölder's inequality, we know that, for any  $p > 3/2$ ,

$$\int_{B_R} \frac{n_\rho(x)}{|x|} \, dx \leq \left(4\pi \frac{p-1}{2p-3}\right)^{(p-1)/p} \|n_\rho\|_{L^p} R^{\frac{2p-3}{p-1}},$$

where  $B_R$  denotes the centered ball of radius  $R$ . Similarly, for any  $p < 3/2$ ,

$$\int_{B_R^c} \frac{n_\rho(x)}{|x|} \, dx \leq \left(4\pi \frac{p-1}{3-2p}\right)^{(p-1)/p} \|n_\rho\|_{L^p} R^{-\frac{2p-3}{p-1}}.$$

Applying these two estimates with, for instance,  $p = 3$  and  $p = 6/5$  and optimizing w.r.t.  $R > 0$ , we obtain a limiting case for the Hardy-Littlewood-Sobolev inequalities after using again Hölder's inequality to estimate  $\|n_\rho\|_{L^{6/5}}$  in terms of  $\|n_\rho\|_{L^1}$  and  $\|n_\rho\|_{L^3}$ :

$$\int_{\mathbb{R}^3} \frac{n_\rho(x)}{|x|} \, dx \leq C \|n_\rho\|_{L^1}^{3/2} \|n_\rho\|_{L^3}^{1/2}.$$

We conclude as in (2.1) using Sobolev's inequality to control  $\|n_\rho\|_{L^3}$  by  $\operatorname{tr}(-\Delta \rho)$ .  $\square$

As a consequence of Proposition 3.1 and Lemma 3.2, we obtain the following result.

**Corollary 3.3** (Binding inequality). *Let  $M^{(1)} > 0$  and  $M^{(2)} > 0$ . If there are minimizers for  $i_{M^{(1)},T}$  and  $i_{M^{(2)},T}$ , then*

$$i_{M^{(1)}+M^{(2)},T} < i_{M^{(1)},T} + i_{M^{(2)},T}.$$

*Proof.* Consider two minimizers  $\rho^{(1)}$  and  $\rho^{(2)}$  for  $i_{M^{(1)},T}$  and  $i_{M^{(2)},T}$  respectively and let  $\chi_R$  be the cut-off function given in (2.2). By Lemma 2.2 we have

$$\operatorname{tr}(-\Delta(\chi_R \rho^{(\ell)} \chi_R)) \leq \operatorname{tr}(-\Delta \rho^{(\ell)}) + O(R^{-2}) \quad \text{and} \quad \operatorname{tr} \beta(\chi_R \rho^{(\ell)} \chi_R) \leq \operatorname{tr} \beta(\rho^{(\ell)}).$$

To handle the potential energies, we observe that

$$\begin{aligned} \left| \mathcal{E}_{\text{pot}}[\chi_R \rho^{(\ell)} \chi_R] - \mathcal{E}_{\text{pot}}[\rho^{(\ell)}] \right| &\leq \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{(1 - \chi_R^2(x) \chi_R^2(y)) n_{\rho^{(\ell)}}(x) n_{\rho^{(\ell)}}(y)}{|x - y|} \, dx \, dy \\ &\leq \iint_{\{|x| \geq R\} \times \{|y| \geq R\}} \frac{n_{\rho^{(\ell)}}(x) n_{\rho^{(\ell)}}(y)}{|x - y|} \, dx \, dy. \end{aligned}$$

Using Lemma 3.1 and Lemma 3.2, we obtain

$$\left| \mathcal{E}_{\text{pot}}[\chi_R \rho^{(\ell)} \chi_R] - \mathcal{E}_{\text{pot}}[\rho^{(\ell)}] \right| \leq C \left[ \text{tr}(-\Delta \rho^{(\ell)}) \right]^{1/2} \int_{|x| \geq R} n_{\rho^{(\ell)}}(x) \, dx \leq O(R^{-2})$$

for  $R > 0$  large enough. This shows that, for any  $R > 0$  sufficiently large

$$\mathcal{F}_T[\chi_R \rho^{(\ell)} \chi_R] \leq i_{M^{(\ell)}, T} + O(R^{-2}) \quad \text{for } \ell = 1, 2.$$

Consider now the test state

$$\rho_R := \chi_R \rho^{(1)} \chi_R + \tau_{5R\mathbf{e}}^* \chi_R \rho^{(2)} \chi_R \tau_{5R\mathbf{e}}$$

for some unit vector  $\mathbf{e} \in \mathbb{S}^2$ . Since  $\|n_{\rho_R}\|_{L^1} \leq M^{(1)} + M^{(2)}$ , by monotonicity of  $M \mapsto i_{M, T}$  (see Proposition 2.3 (ii)), we get

$$\begin{aligned} i_{M^{(1)}+M^{(2)}, T} &\leq \mathcal{F}_T[\rho_R] \leq \mathcal{F}_T[\chi_R \rho^{(1)} \chi_R] + \mathcal{F}_T[\chi_R \rho^{(2)} \chi_R] - \frac{M^{(1)}M^{(2)}}{9R} \\ &\leq i_{M^{(1)}, T} + i_{M^{(2)}, T} + \frac{C}{R^2} - \frac{M^{(1)}M^{(2)}}{9R} \end{aligned}$$

for some positive constant  $C$ , which yields the desired result for  $R$  sufficiently large.  $\square$

#### 4. EXISTENCE OF MINIMIZERS BELOW $T^*$

By a classical result, see e.g. [13, Corollary 4.1], conservation of mass along a weakly convergent minimizing sequence implies that the sequence strongly converges. More precisely, we have the following statement.

**Lemma 4.1.** *Let  $(\rho_k)_{k \in \mathbb{N}} \in \mathfrak{H}_M$  be a minimizing sequence for  $\mathcal{F}_T$ , such that  $\rho_k \rightharpoonup \rho$  weak- $*$  in  $\mathfrak{H}$  and  $n_{\rho_k} \rightarrow n_\rho$  almost everywhere as  $k \rightarrow \infty$ . Then  $\rho_k \rightarrow \rho$  strongly in  $\mathfrak{H}$  if and only if  $\text{tr } \rho = M$ .*

*Proof.* The proof relies on a characterization of the compactness due to Brezis and Lieb (see [1] and [15, Theorem 1.9]) from which it follows that

$$\begin{aligned} \lim_{k \rightarrow \infty} \left( \int_{\mathbb{R}^3} n_{\rho_k} \, dx - \int_{\mathbb{R}^3} |n_\rho - n_{\rho_k}| \, dx \right) &= \int_{\mathbb{R}^3} n_\rho \, dx \\ \text{and } \lim_{k \rightarrow \infty} \left( \text{tr}(-\Delta \rho) - \text{tr}(-\Delta(\rho - \rho_k)) \right) &= \text{tr}(-\Delta \rho). \end{aligned}$$

By semi-continuity of  $\mathcal{F}_T$ , monotonicity of  $M \mapsto i_{M, T}$  according to Proposition 2.3 (ii) and compactness of the quadratic term in  $\mathcal{E}_H$ , we conclude that  $\lim_{k \rightarrow \infty} \text{tr}(-\Delta(\rho - \rho_k)) = 0$  if and only if  $\text{tr } \rho = M$ .  $\square$

With the results of Section 2 in hand, we can now state an existence result for minimizers of  $\mathcal{F}_T$ . To this end, consider a minimizing sequence  $(\rho_n)_{n \in \mathbb{N}}$  for  $\mathcal{F}_T$  and recall that  $(\rho_n)_{n \in \mathbb{N}}$  is said to be *relatively compact up to translations* if there is a sequence  $(a_n)_{n \in \mathbb{N}}$  of points in  $\mathbb{R}^3$  such that  $\tau_{a_n}^* \rho_n \tau_{a_n}$  strongly converges as  $n \rightarrow \infty$ , up to the extraction of subsequences.

Clearly, the sub-additivity inequality given in Lemma 2.3 (i) is not sufficient to prove the compactness up to translations for  $(\rho_n)_{n \in \mathbb{N}}$ . More precisely, if *equality* holds, then, as in the proof of Lemma 2.3, one can construct a minimizing sequence that is *not* relatively compact in  $\mathfrak{H}$  up to translations. This obstruction is usually referred to as *dichotomy*, cf. [18]. To overcome this difficulty, we shall rely on the strict sub-additivity of Corollary 3.3, which, however, only holds for minimizers. This is the main difference with previous works on Hartree-Fock models.

As we shall see, the main issue will therefore be to prove the convergence of two subsequences towards minimizers of mass smaller than  $M$ .

**Proposition 4.2.** *Assume that  $(\beta 1)$ – $(\beta 3)$  hold. Let  $M > 0$  and consider  $T^* = T^*(M)$  defined by (1.8). For all  $T < T^*$ , there exists an operator  $\rho$  in  $\mathfrak{H}_M$  such that  $\mathcal{F}_T[\rho] = i_{M,T}$ . Moreover, every minimizing sequence  $(\rho_n)_{n \in \mathbb{N}}$  for  $i_{M,T}$  is relatively compact in  $\mathfrak{H}$  up to translations.*

*Proof.* The proof is based on the concentration-compactness method as in [13]. Compared to previous results (see for instance [20, 21, 22, 13]), the main difficulty arises in the splitting case, as we shall see below.

*Step 1: Non-vanishing.* We split

$$\mathcal{E}_{\text{pot}}[\rho_n] = \iint_{\mathbb{R}^6} \frac{n_{\rho_n}(x) n_{\rho_n}(y)}{|x - y|} dx dy$$

into three integrals  $I_1$ ,  $I_2$  and  $I_3$  corresponding respectively to the domains  $|x - y| < 1/R$ ,  $1/R < |x - y| < R$  and  $|x - y| > R$ , for some  $R > 1$  to be fixed later. Since  $n_{\rho_n}$  is bounded in  $L^1(\mathbb{R}^3) \cap L^3 \subset L^{7/5}(\mathbb{R}^3)$  by Lemma 2.1, by Young's inequality we can estimate  $I_1$  by

$$I_1 \leq \|n_{\rho_n}\|_{L^{7/5}}^2 \| |\cdot|^{-1} \|_{L^{7/4}(B_{1/R})} \leq \frac{C}{R^{5/7}},$$

and directly get bounds on  $I_2$  and  $I_3$  by computing

$$\begin{aligned} I_2 &\leq R \iint_{|x-y| < R} n_{\rho_n}(x) n_{\rho_n}(y) dx dy \leq R M \sup_{y \in \mathbb{R}^3} \int_{y+B_R} n_{\rho_n}(x) dx, \\ I_3 &\leq \frac{1}{R} \iint_{\mathbb{R}^6} n_{\rho_n}(x) n_{\rho_n}(y) dx dy \leq \frac{M^2}{R}. \end{aligned}$$

Keeping in mind that  $i_{M,T} < 0$ , we have

$$\mathcal{F}_T[\rho_n] \geq i_{M,T} > -I_1 - I_2 - I_3$$

for any  $n$  large enough, which proves the *non-vanishing* property:

$$\lim_{n \rightarrow \infty} \int_{a_n+B_R} n_{\rho_n}(x) dx \geq \frac{1}{RM} \left( -i_{M,T} - \frac{M^2}{R} - \frac{C}{R^{5/7}} \right) > 0$$

for  $R$  big enough and for some sequence  $(a_n)_{n \in \mathbb{N}}$  of points in  $\mathbb{R}^3$ . Replacing  $\rho_n$  by  $\tau_{a_n}^* \rho_n \tau_{a_n}$  and denoting by  $\rho^{(1)}$  the weak limit of  $(\rho_n)_{n \in \mathbb{N}}$  (up to the extraction of a subsequence), we have proved that  $M^{(1)} = \int_{\mathbb{R}^3} n_{\rho^{(1)}} dx > 0$ .

*Step 2: Dichotomy.* Either  $M^{(1)} = M$  and  $\rho_n$  strongly converges to  $\rho$  in  $\mathfrak{H}$  by Lemma 4.1, or  $M^{(1)} \in (0, M)$ . Let us choose  $R_n$  such that  $\int_{\mathbb{R}^3} n_{\rho_n^{(1)}} dx = M^{(1)} + (M - M^{(1)})/n$  where  $\rho_n^{(1)} := \chi_{R_n} \rho_n \chi_{R_n}$ . Let  $\rho_n^{(2)} := \xi_{R_n} \rho_n \xi_{R_n}$ . By definition of  $R_n$ ,  $\lim_{n \rightarrow \infty} R_n = \infty$ . By Step 1, we know that  $\rho_n^{(1)}$  strongly converges to  $\rho^{(1)}$ . By Identity (2.3) and Lemma 2.2, we find that

$$\mathcal{F}_T[\rho_n] \geq \mathcal{F}_T[\rho_n^{(1)}] + \mathcal{F}_T[\rho_n^{(2)}] + O(R_n^{-2}) - \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{n_{\rho_n^{(1)}}(x) n_{\rho_n^{(2)}}(y)}{|x - y|} dx dy,$$

thus showing that

$$i_{M,T} = \lim_{n \rightarrow \infty} \mathcal{F}_T[\rho_n] \geq \mathcal{F}_T[\rho^{(1)}] + \lim_{n \rightarrow \infty} \mathcal{F}_T[\rho_n^{(2)}].$$

By step 1,  $\lim_{n \rightarrow \infty} \int_{\mathbb{R}^3} n_{\rho_n^{(2)}} dx = M - M^{(1)}$ . By sub-additivity, according to Lemma 2.3 (i),  $\rho^{(1)}$  is a minimizer for  $i_{M^{(1)},T}$ ,  $(\rho_n^{(2)})_{n \in \mathbb{N}}$  is a minimizing sequence for  $i_{M-M^{(1)},T}$  and

$$i_{M,T} = i_{M^{(1)},T} + i_{M-M^{(1)},T}.$$

Either  $i_{M-M^{(1)},T} = 0$  and then  $i_{M,T} = i_{M-M^{(1)},T}$ , which contradicts Corollary 2.6, and the assumption  $T < T^*$ , or  $i_{M-M^{(1)},T} < 0$ . In this case, we can reapply the previous analysis to  $(\rho_n^{(2)})_{n \in \mathbb{N}}$  and get that for some  $M^{(2)} > 0$ ,  $(\rho_n^{(2)})_{n \in \mathbb{N}}$  converges up to a translation to a minimizer  $\rho^{(2)}$  for  $i_{M^{(2)},T}$  and

$$i_{M,T} = i_{M^{(1)},T} + i_{M^{(2)},T} + i_{M-M^{(1)}-M^{(2)},T}.$$

From Corollary 3.3 and 2.3 (i), we get respectively  $i_{M^{(1)}+M^{(2)},T} < i_{M^{(1)},T} + i_{M^{(2)},T}$  and  $i_{M^{(1)}+M^{(2)},T} + i_{M-M^{(1)}-M^{(2)},T} \leq i_{M,T}$ , a contradiction.  $\square$

As a direct consequence of the variational approach, the set of minimizers  $\mathfrak{M}_M$  is *orbitally stable* under the dynamics of (1.4). To quantify this stability, define

$$\text{dist}_{\mathfrak{M}_M}(\sigma) := \inf_{\rho \in \mathfrak{M}_M} \|\rho - \sigma\|_{\mathfrak{H}}.$$

**Corollary 4.3.** *Assume that  $(\beta 1)$ – $(\beta 3)$  hold. For any given  $M > 0$ , let  $T \in (0, T^*(M))$ . For any  $\varepsilon > 0$ , there exists  $\delta > 0$  such that, for all  $\rho_{\text{in}} \in \mathfrak{H}_M$  with  $\text{dist}_{\mathfrak{M}_M}(\rho_{\text{in}}) \leq \delta$ ,*

$$\sup_{t \in \mathbb{R}_+} \text{dist}_{\mathfrak{M}_M}(\rho(t)) \leq \varepsilon$$

where  $\rho(t)$  is the solution of (1.4) with initial data  $\rho_{\text{in}} \in \mathfrak{H}_M$ .

Similar results have been established in many earlier papers like, for instance in [24] in the case of repulsive Coulomb interactions. As in [4, 24], the result is a direct consequence of the conservation of the free energy along the flow and the compactness of all minimizing sequences. According to [14], for  $T \in (0, T_c]$ , the minimizer corresponding to  $i_{M,T}$  is unique up to translations (see next Section). A much stronger stability result can easily be achieved. Details are left to the reader.

## 5. CRITICAL TEMPERATURE FOR MIXED STATES

In this subsection, we shall deduce the existence a critical temperature  $T_c \in (0, T^*)$ , above which minimizers  $\rho \in \mathfrak{M}_M$  become true mixed states, i.e. density matrix operators with rank higher than one.

**Lemma 5.1.** *For all  $M > 0$ , the map  $T \mapsto i_{M,T}$  is concave.*

*Proof.* Fix some  $T_0 > 0$  and write

$$\mathcal{F}_T[\rho] = \mathcal{F}_{T_0}[\rho] + (T - T_0) |\mathcal{S}[\rho]|.$$

Denoting by  $\rho_{T_0}$  the minimizer for  $\mathcal{F}_{T_0}$ , we obtain

$$i_{M,T} \leq i_{M,T_0} + (T - T_0) |\mathcal{S}[\rho_{T_0}]|$$

which means that  $|\mathcal{S}[\rho_{T_0}]|$  lies in the cone tangent to  $T \mapsto i_{M,T}$  and  $i_{M,T}$  lies below it, i.e.  $T \mapsto i_{M,T}$  is concave.  $\square$

Consider  $T_c$  defined by (1.9), i.e. the largest possible  $T_c$  such that  $i_{M,T} = i_{M,0} + T\beta(M)$  for  $T \in [0, T_c]$  and recall some results concerning the zero temperature case. Lieb in [14] proved that  $\mathcal{F}_{T=0} = \mathcal{E}_H$  has a unique radial minimizer  $\rho_0 = M|\psi_0\rangle\langle\psi_0|$ . The corresponding Hamiltonian operator

$$(5.1) \quad H_0 := -\Delta - |\psi_0|^2 * |\cdot|^{-1} = H_{\rho_0}$$

admits countably many negative eigenvalues  $(\mu_j^{(0)})_{j \in \mathbb{N}}$ , which accumulate at zero. We shall use these eigenvalues to characterize the critical temperature  $T_c$ . To this end we need the following lemma.

**Lemma 5.2.** *Assume that  $(\beta 1)$ – $(\beta 3)$  hold. With  $T_c$  defined by (1.9),  $T_c(M)$  is positive for any  $M > 0$ .*

*Proof.* Consider a sequence  $(T_n)_{n \in \mathbb{N}} \in \mathbb{R}_+$  such that  $\lim_{n \rightarrow \infty} T_n = 0$ . Let  $\rho^{(n)} \in \mathfrak{M}_M$  denote the associated sequence of minimizers with occupation numbers  $(\lambda_j^{(n)})_{j \in \mathbb{N}}$ . According to (2.8), we know that

$$\lambda_j^{(n)} = (\beta')^{-1} \left( (\mu^{(n)} - \mu_j^{(n)})/T_n \right) \quad \forall j \in \mathbb{N},$$

where, for any  $n \in \mathbb{N}$ ,  $(\mu_j^{(n)})_{j \in \mathbb{N}}$  denotes the sequence of eigenvalues of  $H_{\rho^{(n)}}$  and  $\mu^{(n)} \leq 0$  is the associated chemical potential. Since  $\rho^{(n)}$  is a minimizing sequence for  $\mathcal{F}_{T=0}$ , we know that

$$\lim_{n \rightarrow \infty} \mu_j^{(n)} = \mu_j^0 \leq 0$$

where  $(\mu_j^0)_{j \in \mathbb{N}}$  are the eigenvalues of  $H_0$ . Arguing by contradiction, we assume that

$$\liminf_{n \rightarrow \infty} \lambda_1^{(n)} = \epsilon > 0.$$

By (2.8) and the fact that  $\beta'$  is increasing, this implies:  $\mu^{(n)} > \mu_1^{(n)} \rightarrow \mu_1^0$  as  $n \rightarrow \infty$ . Then

$$M = \lambda_0^0 \geq \lim_{n \rightarrow \infty} \lambda_0^{(n)} = \lim_{n \rightarrow \infty} (\beta')^{-1} \left( \frac{\mu^{(n)} - \mu_0^{(n)}}{T_n} \right) \geq \lim_{n \rightarrow \infty} (\beta')^{-1} \left( \frac{\mu_1^0 - \mu_0^{(n)}}{T_n} \right) = +\infty.$$

This proves that there exists an interval  $[0, T_c)$  with  $T_c > 0$  such that, for any  $T_n \in [0, T_c)$ , it holds  $\mu^{(n)} < \mu_1^{(n)}$ , and, as a consequence,  $\rho^{(n)}$  is of rank one. Hence, for any  $T \in [0, T_c)$ , the minimizer of  $\mathcal{F}_T$  in  $\mathfrak{H}_M$  is also a minimizer of  $\mathcal{E}_H + T\beta(M)$ . From [14], we know that it is unique and given by  $\rho_0$ , in which case  $i_{M,T} = i_{M,0} - T\mathcal{S}[\rho_0] = i_{M,0} + T\beta[M]$ .  $\square$

As an immediate consequence of Lemmata 5.1 and 5.2 we obtain the following corollary.

**Corollary 5.3.** *Assume that  $(\beta 1)$ – $(\beta 3)$  hold. There is a pure state minimizer of mass  $M$  if and only if  $T \in [0, T_c]$ .*

*Proof.* A pure state satisfies  $i_{M,T} = i_{M,0} + T\beta(M)$  and from the concavity property stated in Lemma 5.1 we conclude  $i_{M,T} < i_{M,0} + T\beta(M)$  for all  $T > T_c$ .  $\square$

We finally give a characterization of  $T_c$ .

**Proposition 5.4.** *Assume that  $(\beta 1)$ – $(\beta 3)$  hold. For any  $M > 0$ , the critical temperature satisfies*

$$T_c(M) = \frac{\mu_1^0 - \mu_0^0}{\beta'(M)},$$

where  $\mu_0^0$  and  $\mu_1^0$  are the two lowest eigenvalues of  $H_0$  defined in (5.1).

*Proof.* For  $T \leq T_c$ , there exists a unique pure state minimizer  $\rho_0$ . For such a pure state, the Lagrange multiplier associated to the mass constraint  $\text{tr } \rho_0 = M$  is given by  $\mu = \mu(T)$ . According to 2.7, it is given by  $T \beta'(M) + \mu_0^0 - \mu(T) = 0$  for any  $T < T_c$  (as long as the minimizer is of rank one). This uniquely determines  $\mu(T)$ . On the other hand we know that  $0 \neq \lambda_1 = (\beta')^{-1}((\mu_1^0 - \mu(T))/T)$  if  $T > (\mu_1^0 - \mu_0^0)/\beta'(M)$ , thus proving that  $T_c \leq (\mu_1^0 - \mu_0^0)/\beta'(M)$ .

It remains to prove equality: By using Lemmas 5.1 and 5.2, we know that  $i_{M,T_c} = i_{M,0} + T_c \beta(M)$ . Let  $\rho$  be a minimizer for  $T = T_c$ . The two inequalities,  $i_{M,0} \leq \mathcal{E}_H[\rho]$  and  $\beta(M) \leq \text{tr } \beta(\rho)$  hold as equalities if and only if, in both cases,  $\rho$  is of rank one. Consider a sequence  $(T^{(n)})_{n \in \mathbb{N}}$  such that  $\lim_{n \rightarrow \infty} T^{(n)} = T_c$ ,  $T^{(n)} > T_c$  for any  $n \in \mathbb{N}$  and, if  $(\rho^{(n)})_{n \in \mathbb{N}}$  denotes a sequence of associated minimizers with  $(\mu_j^{(n)})_{j \in \mathbb{N}}$  and  $\mu^{(n)} \leq 0$  as in the proof of Lemma 5.2, we have  $\mu^{(n)} > \mu_1^{(n)}$  so that  $\lambda_1^{(n)} > 0$  for any  $n \in \mathbb{N}$ . The sequence  $(\rho^{(n)})_{n \in \mathbb{N}}$  is minimizing for  $i_{M,T_c}$ , thus proving that  $\lim_{n \rightarrow \infty} \lambda_1^{(n)} = 0$ , so that  $\lim_{n \rightarrow \infty} \mu^{(n)} = \mu_1^0$ . Passing to the limit in

$$M \mu^{(n)} = \sum_{j \in \mathbb{N}} \lambda_j^{(n)} \left( \mu_j^{(n)} + T^{(n)} \beta'(\lambda_j^{(n)}) \right)$$

completes the proof.  $\square$

## 6. ESTIMATES ON THE MAXIMAL TEMPERATURE

All above results require  $T < T^*$ , the maximal temperature. In some situations, we can prove that  $T^*$  is finite.

**Proposition 6.1.** *Let  $\beta(s) = s^p$  with  $p \in (1, 7/5)$ . Then, for any  $M > 0$ , the maximal temperature  $T^* = T^*(M)$  is finite.*

*Proof.* Let  $V$  be a given non-negative potential. From [7], we know that

$$2T \text{tr } \beta(\rho) + \text{tr}(-\Delta \rho) - \text{tr}(V\rho) \geq -(2T)^{-\frac{1}{p-1}} (p-1) p^{-\frac{p}{p-1}} \sum_j |\mu_j(V)|^\gamma$$

where  $\gamma = \frac{p}{p-1}$  and  $\mu_j(V)$  denotes the negative eigenvalues of  $-\Delta - V$ . The sum is extended to all such eigenvalues. By the Lieb-Thirring inequality, we have the estimate

$$\sum_j |\mu_j(V)|^\gamma \leq C_{\text{LT}}(\gamma) \int_{\mathbb{R}^3} |V|^q dx$$

with  $q = \gamma + \frac{3}{2}$ . In summary, this amounts to

$$2T \text{tr } \beta(\rho) + \text{tr}(-\Delta \rho) - \text{tr}(V\rho) \geq -(2T)^{-\frac{1}{p-1}} (p-1) p^{-\frac{p}{p-1}} C_{\text{LT}}(\gamma) \int_{\mathbb{R}^3} |V|^q dx.$$

Applying the above inequality to  $V = V_\rho = n_\rho * |\cdot|^{-1}$ , we find that

$$\begin{aligned} \mathcal{F}_T[\rho] &= \frac{1}{2} \text{tr}(-\Delta \rho) + \frac{1}{2} \left[ (2T) \text{tr } \beta(\rho) + \text{tr}(-\Delta \rho) - \text{tr}(V_\rho \rho) \right] \\ &\geq \frac{1}{2} \text{tr}(-\Delta \rho) - T^{-\frac{1}{p-1}} (2p)^{-\frac{p}{p-1}} C_{\text{LT}}(\gamma) \int_{\mathbb{R}^3} |V_\rho|^q dx. \end{aligned}$$

Next, we invoke the Hardy-Littlewood-Sobolev inequality

$$\int_{\mathbb{R}^3} |V_\rho|^q dx \leq C_{\text{HLS}} \|n_\rho\|_{L^r(\mathbb{R}^3)}^q$$



for some  $r > 1$  such that  $\frac{1}{r} = \frac{2}{3} + \frac{1}{q}$ . Notice that  $r > 1$  means  $q > 3$  and hence  $p < 3$ . Hölder's inequality allows to estimate the right hand side by

$$\|n_\rho\|_{L^r(\mathbb{R}^3)} \leq \|n_\rho\|_{L^1(\mathbb{R}^3)}^\theta \|n_\rho\|_{L^3(\mathbb{R}^3)}^{1-\theta}$$

with  $\theta = \frac{3}{2}(\frac{1}{r} - \frac{1}{3})$ . Since  $\|n_\rho\|_{L^3(\mathbb{R}^3)}$  is controlled by  $\|\nabla \sqrt{n_\rho}\|_{L^2}^2$  using Sobolev's embedding, which is itself bounded by  $\text{tr}(-\Delta \rho)$ , we conclude that

$$\int_{\mathbb{R}^3} |V_\rho|^q dx \leq c M^{q\theta} (\text{tr}(-\Delta \rho))^{q(1-\theta)}$$

for some positive constant  $c$  and, as a consequence,

$$(6.1) \quad \mathcal{F}_T[\rho] \geq \frac{1}{2} \text{tr}(-\Delta \rho) - T^{-\frac{1}{p-1}} K \text{tr}(-\Delta \rho)^{q(1-\theta)},$$

for some  $K > 0$ . Moreover we find that

$$q(1-\theta) = 1 + \eta \quad \text{with} \quad \eta = \frac{7-5p}{4(p-1)},$$

so that  $\eta$  is positive if  $p \in (1, 7/5)$ .

Assume that  $i_{M,T} < 0$  and consider an admissible  $\rho \in \mathfrak{H}_M$  such that  $\mathcal{F}_T[\rho] = i_{M,T}$ . Since  $\text{tr} \beta(\rho)$  is positive, as in the proof of (2.1), we know that for some positive constant  $C$ , which is independent of  $T > 0$ ,

$$0 > \mathcal{F}_T[\rho] > \mathcal{E}_H[\rho] \geq \text{tr}(-\Delta \rho) - C M^{3/2} \text{tr}(-\Delta \rho)^{\frac{1}{2}},$$

and, as a consequence,

$$\text{tr}(-\Delta \rho) \leq C^2 M^3.$$

On the other hand, by (6.1), we know that  $\mathcal{F}_T[\rho] < 0$  means that

$$\text{tr}(-\Delta \rho) > \left( \frac{T^{\frac{1}{p-1}}}{2K} \right)^{\frac{1}{\eta}}.$$

The compatibility of these two conditions amounts to

$$T^{\frac{1}{p-1}} \leq 2K C^{2\eta} M^{3\eta},$$

which provides an upper bound for  $T^*(M)$ . □

Finally, we infer the following asymptotic property for the infimum of  $\mathcal{F}_T[\rho]$ .

**Lemma 6.2.** *Assume that (β1)–(β2) hold. If  $T^* < +\infty$ , then  $\lim_{T \rightarrow T_-^*} i_{M,T} = 0$ .*

*Proof.* The proof follows from the concavity of  $T \mapsto i_{M,T}$  (see Lemma 5.1). Let  $\rho_{T_0}$  denote the minimizer at  $T_0 < T^*$ , with  $\mathcal{F}_{T_0}[\rho_{T_0}] = -\delta$  for some  $\delta > 0$ . Then we observe

$$i_{M,T} \leq (T - T_0) \sum_{j \in \mathbb{N}} \beta(\lambda_j) + \mathcal{F}_{T_0}[\rho_{T_0}] \leq (T - T_0) \beta(M) - \delta < 0,$$

for all  $T$  such that:  $T - T_0 \leq \delta/\beta(M)$ , which is in contradiction with the definition of  $T^*$  given in (1.8) if  $\liminf_{T \rightarrow T_-^*} i_{M,T} < 0$ . □

## 7. CONCLUDING REMARKS

Assumption  $(\beta 3)$  is needed for Corollary 2.6, which is used itself in the proof of Proposition 4.2 (compactness of minimizing sequences). When  $\beta(s) = s^p$ , this means that we have to introduce the restriction  $p \leq 3$ . If look at the details of the proof, what is really needed is that  $\mu = \frac{\partial i_{M,T}}{\partial M}$  takes negative values. To further clarify the role of the threshold  $p = 3$ , we can state the following result.

**Proposition 7.1.** *Assume that  $\beta(s) = s^p$  for some  $p > 1$ . Then we have*

$$(7.1) \quad M \frac{\partial i_{M,T}}{\partial M} + (3-p) T \frac{\partial i_{M,T}}{\partial T} \leq 3 i_{M,T}$$

and, as a consequence:

- (i) if  $p \leq 3$ , then  $i_{M,T} \leq (\frac{M}{M_0})^3 i_{M,T_0}$  for any  $M > M_0 > 0$  and  $T > 0$ .
- (ii) if  $p \geq 3$ , then  $i_{M,T} \leq (\frac{T}{T_0})^{3/(3-p)} i_{M,T_0}$  for any  $M > 0$  and  $T > T_0 > 0$ .

*Proof.* Let  $\rho \in \mathfrak{H}_M$  and, using the representation (1.1), define

$$\rho_\lambda := \lambda^4 \sum_{j \in \mathbb{N}} \lambda_j |\psi_j(\lambda \cdot)\rangle \langle \psi_j(\lambda \cdot)|.$$

With  $M[\rho] := \text{tr } \rho = \int_{\mathbb{R}^3} n_\rho dx$ , we find that

$$M[\rho_\lambda] = \lambda M[\rho] = \lambda M$$

and

$$\mathcal{F}_{\lambda^{3-p} T}[\rho_\lambda] = \lambda^3 \mathcal{F}_T[\rho].$$

As a consequence, we have

$$i_{\lambda M, \lambda^{3-p} T} \leq \lambda^3 i_{M,T},$$

which proves (7.1) by differentiating at  $\lambda = 1$ . In case (i), since  $T \mapsto i_{M,T}$  is non-decreasing, we have

$$i_{\lambda M_0, T} \leq i_{\lambda M_0, \lambda^{3-p} T} \leq \lambda^3 i_{M_0, T} \quad \forall \lambda > 1$$

and the conclusion holds with  $\lambda = M/M_0$ . In case (ii), since  $M \mapsto i_{M,T}$  is non-increasing, we have

$$i_{M, \lambda^{3-p} T_0} \leq i_{\lambda M, \lambda^{3-p} T_0} \leq \lambda^3 i_{M, T_0} \quad \forall \lambda \in (0, 1)$$

and the conclusion holds with  $\lambda = (T/T_0)^{1/(3-p)}$ .  $\square$

Assume that  $\beta(s) = s^p$  for any  $s \in \mathbb{R}^+$ . We observe that for  $T < T^*(M)$ ,  $\frac{\partial i_{M,T}}{\partial M} \leq \frac{3}{M} i_{M,T}$  if  $p \leq 3$ , but we have no such estimate if  $p > 3$ . In Proposition 2.3 (iii), the sufficient condition for showing that  $T^*(M) = \infty$  is precisely  $p > 3$ . Hence, at this stage, we do not have an example of a function  $\beta$  satisfying Assumptions  $(\beta 1)$  and  $(\beta 2)$  for which existence of a minimizer of  $i_{M,T}$  in  $\mathfrak{H}_M$  is granted for any  $M > 0$  and any  $T > 0$ . In other words, with  $T^*$  can be infinite for a well chosen function  $\beta$ , for instance  $\beta(s) = s^p$ ,  $s \in \mathbb{R}^+$ , for  $p > 3$ . However, in such a case we do not know if the Lagrange multiplier  $\mu(T)$  is negative for any  $T > 0$  and as a consequence, the existence of a minimizer corresponding to  $i_{M,T}$  is an open question for large values of  $T$ .

## APPENDIX A. PROOF OF PROPOSITION 3.1

Consider the minimizer  $\rho$  of Proposition 3.1 and let  $\mu < 0$  be the Lagrange multiplier corresponding to the mass constraint  $\text{tr } \rho = M$ . Define

$$\mathcal{G}_T^\mu[\rho] := \mathcal{F}_T[\rho] - \mu \text{tr}(\rho) .$$

The density operator  $\rho$  is a minimizer of the unconstrained minimization problem  $\inf_{\rho \in \mathfrak{H}} \mathcal{G}_T^\mu[\rho]$ . By the same argument as in the proof of Proposition 2.4 we know that  $\rho$  also solves the linearized minimization problem  $\inf_{\sigma \in \mathfrak{H}} \mathcal{L}^\mu[\sigma]$  where

$$\mathcal{L}^\mu[\sigma] := \text{tr} [(H_\rho - \mu + T \beta'(\rho)) \sigma] .$$

Consider the cut-off functions  $\chi_R$  and  $\xi_R$  defined in (2.2) and let  $\rho_R := \chi_R \rho \chi_R$ . By Lemma 2.2, we know that, as  $R \rightarrow \infty$ ,

$$\text{tr}(-\Delta \rho) \geq \text{tr}(-\Delta \rho_R) + \text{tr}(-\Delta (\xi_R \rho \xi_R)) - \frac{C}{R^2}$$

for some positive constant  $C$ . Next we rewrite the potential energy as

$$\begin{aligned} \mathcal{E}_{\text{pot}}[\rho] &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{n_\rho(x) \chi_R^2(y) n_\rho(y)}{|x-y|} dx dy + \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\chi_{R/4}^2(x) n_\rho(x) \xi_R^2(y) n_\rho(y)}{|x-y|} dx dy \\ &\quad + \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\xi_{R/4}^2(x) n_\rho(x) \xi_R^2(y) n_\rho(y)}{|x-y|} dx dy . \end{aligned}$$

In the second integral we use the fact that  $|x-y| \geq R/2$ , whereas the third integral can be estimated by Lemma 3.2. Using the fact that

$$\begin{aligned} \varepsilon(R) &:= \text{tr}(-\Delta (\xi_R \rho \xi_R)) \\ &= \sum_{j \in \mathbb{N}} \lambda_j \int_{\mathbb{R}^3} |\nabla (\xi_R \psi_j)|^2 dx \leq 2 \frac{M}{R^2} \|\nabla \xi\|_{L^\infty}^2 + 2 \sum_{j \in \mathbb{N}} \lambda_j \int_{\mathbb{R}^3} \xi_R^2 |\nabla \psi_j|^2 dx \end{aligned}$$

converges to 0 as  $R \rightarrow \infty$ , we obtain that  $\|\xi_{R/4}^2 n_\rho * |\cdot|^{-1}\|_{L^\infty} \leq C \sqrt{\varepsilon(R/4)} \rightarrow 0$  and can estimate the third integral by

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\xi_{R/4}^2(x) n_\rho(x) \xi_R^2(y) n_\rho(y)}{|x-y|} dx dy \leq C \sqrt{\varepsilon(R/4)} \int_{\mathbb{R}^3} \xi_R^2(y) n_\rho(y) dx .$$

In summary this yields

$$\mathcal{E}_{\text{pot}}[\rho] \leq \text{tr}(V_\rho \rho_R) + o(1) \int_{\mathbb{R}^3} \xi_R^2 n_\rho dx .$$

Collecting all estimates, we have proved that

$$\mathcal{L}^\mu[\rho_R] \leq \mathcal{L}^\mu[\rho] - \varepsilon(R) + (\mu + o(1)) \int_{\mathbb{R}^3} \xi_R^2 n_\rho dx + \frac{C}{R^2}$$

as  $R \rightarrow \infty$ . Recall that  $\varepsilon(R)$  is non-negative,  $\mu$  is negative (by Lemma 2.5) and  $\rho$  is a minimizer of  $\mathcal{L}^\mu$  so that  $\mathcal{L}^\mu[\rho] \leq \mathcal{L}^\mu[\rho_R]$ . As a consequence,

$$(\mu + o(1)) \int_{\mathbb{R}^3} \xi_R^2 n_\rho dx + \frac{C}{R^2} \geq 0$$

for  $R$  large enough, which completes the proof of Proposition 3.1.  $\square$

*Acknowledgments.* The authors thank P. Markowich and G. Rein for helpful discussions.

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(G.L. Aki) FACULTY OF MATHEMATICS, UNIVERSITY OF VIENNA, NORDBERGSTRASSE 15, A-1090 VIENNA, AUSTRIA

*E-mail address:* gonca.aki@univie.ac.at

(J. Dolbeault) CEREMADE (UMR CNRS NO. 7534), UNIVERSITÉ PARIS-DAUPHINE, PLACE DE LATRE DE TASSIGNY, F-75775 PARIS CÉDEX 16, FRANCE

*E-mail address:* dolbeaul@ceremade.dauphine.fr

(C. Sparber) DEPARTMENT OF MATHEMATICS, STATISTICS, AND COMPUTER SCIENCE, M/C 249, UNIVERSITY OF ILLINOIS AT CHICAGO, 851 S. MORGAN STREET, CHICAGO, IL 60607, USA

*E-mail address:* sparber@math.uic.edu