Thermal effects in gravitational Hartree systems

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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.

Keywords. Gravitation, Hartree energy, entropy, ground states, free energy, Casimir functional, pure states, mixed states.

1. Introduction

In this paper we investigate the *non-relativistic gravitational Hartree system*. 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 ρ can be decomposed as

$$\rho = \sum_{j \in \mathbb{N}} \lambda_j \, |\psi_j\rangle\langle\psi_j| \tag{1}$$

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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. [37]. 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

$$\int_{\mathbb{R}^3} n_\rho(x) \, \mathrm{d}x = M \, , \tag{2}$$

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

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

where V_ρ 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) for ρ, the Hartree energy can be rewritten as

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

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

$$\mathcal{F}_T[\rho] := \mathcal{E}_H[\rho] - T\,\mathcal{S}[\rho] \tag{3}$$

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

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

The *entropy generating function* β 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

$$i\,\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \left[H_{\rho(t)}, \rho(t)\right] \, , \quad \rho(0) = \rho_{\mathrm{in}} \, . \tag{4}$$

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

$$H_\rho := -\Delta - n_\rho * \frac{1}{|\cdot|} \, . \tag{5}$$

Using again the decomposition (1), this can equivalently be rewritten as a system of (at most) countably many Schrödinger equations coupled through the mean field potential V_ρ:

$$\begin{cases} i\,\partial_t \psi_j + \Delta\,\psi_j + V(t,x)\,\psi_j = 0\,, \quad j \in \mathbb{N}\,, \\ -\Delta V_\rho \,=\, 4\pi \sum_{j\in\mathbb{N}} \lambda_j\,|\psi_j(t,x)|^2\,. \end{cases} \tag{6}$$

This system is a generalization of the gravitational Hartree equation (also known as the *Schrödinger-Newton model*, see [7]) to the case of mixed states. Notice that it reduces to a finite system as soon as only a finite number of λ_j are non-zero. In such a case, ρ 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 [17]. 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 (4) or, equivalently, (6). In the case of *repulsive* self-consistent interactions, describing e.g. electrons, this has been successfully carried out in [8, 9, 10, 26]. In addition, existence of stationary solutions in the repulsive case has been obtained in [25, 28, 29, 30] 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 [16, 19, 21] and, more recently, in [7]. Most of these works rely on the so-called *concentration-compactness method* introduced by Lions in [20]. According to [16], 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 [15] 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 [39, 40, 41, 32, 33, 36, 11, 34, 35]. 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 [26, 9, 10, 8].

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 [16, 19, 21, 7] 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 β. 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. [18, 13, 15]. Moreover, depending on the choice of β, 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

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

and consider the norm

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

The set $\mathfrak{H}$ can be interpreted as the cone of nonnegative density matrix operators with finite energy. Using the decomposition (1), 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 (2) we define the set of physical states by

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

We denote the infimum of the free energy functional $\mathcal{F}_T$, defined in (3), by

$$i_{M,T} = \inf_{\rho \in \mathfrak{H}_M} \mathcal{F}_T[\rho]\,. \tag{7}$$

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

$$T^*(M) := \sup\{T > 0 \ : \ i_{M,T} < 0\}\,. \tag{8}$$

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

(β1) β is strictly convex and of class C^1 on $[0, \infty)$,

(β2) $\beta \geq 0$ on $[0, 1]$ and $\beta(0) = \beta'(0) = 0$,

(β3) $\sup_{m \in (0,\infty)} \frac{m\,\beta'(m)}{\beta(m)} \leq 3$.

A typical example for the function β 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. [12, 33, 34, 39, 40, 41], 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 [23] 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 [16] 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

$$T_c(M) := \max\big\{T > 0 \ : \ i_{M,T} = i_{M,0} + \tau\,\beta(M)\ \forall\,\tau \in (0,T]\,\big\}\,. \tag{9}$$

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 (β1)–(β3) hold. Then, the maximal temperature T^* defined in* (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 ρ solves the self-consistent equation*

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

where H_ρ is the mean-field Hamiltonian defined in (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* (4).

(iii) *The critical temperature T_c defined in* (9) *satisfies $0 < T_c < T^*$ 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 [8] and [15], with differences due to, respectively, the sign of the interaction potential and non-zero temperature effects. The connection between the ρ given in assertion (i) and stationary solutions to (4) will be discussed in more detail in Section 2.3 below, see in particular equation (17). Finally, we note that for $T \in [0, T_c]$, minimizers are reduced to the pure state case for which uniqueness has been proved in [16] (also see [14]). However, uniqueness of minimizers (up to translations and rotations) for $T > T_c$ remains an open question.

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 $T \to T^* < +\infty$. 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 (3) is well defined and $i_{M,T} > -\infty$.

Lemma 2.1. *Assume that (β1)–(β2) 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 $\mathcal{E}_{\rm pot}[\rho]$ can be bounded in terms of the kinetic energy. To this end, note that for every $\rho \in \mathfrak{H}$ we have

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

by the Hardy-Littlewood-Sobolev inequality, see [17, Section 4.3]. Next, by using Sobolev's embedding, we know that $\|n_\rho\|_{L^3}$ is controlled by $\|\nabla \sqrt{n_\rho}\|_{L^2}^2$ which, in view of (1), is bounded by $\operatorname{tr}(-\Delta\, \rho)$. Hence we can conclude that

$$\mathcal{E}_{\rm pot}[\rho] \leq C \, \|n_\rho\|_{L^1}^{3/2} \, \operatorname{tr}(-\Delta\, \rho)^{1/2} \tag{10}$$

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

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

uniformly w.r.t. $\rho \in \mathcal{H}_M$, thus establishing a lower bound on $i_{M,T}$. For the entropy term $\mathcal{S}[\rho] = -\operatorname{tr}\beta(\rho)$ we observe that, since β 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 $\mathfrak{H}_M$. □

Throughout this work, we shall use smooth *cut-off functions* defined as follows. Let χ 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 χ_R and ξ_R by

$$\chi_R(x) = \chi(x/R) \quad \text{and} \quad \xi_R(x) = \sqrt{1 - \chi(x/R)^2} \quad \forall\, x \in \mathbb{R}^3\,. \tag{11}$$

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

$$\int_{\mathbb{R}^3} |u|^2\,\mathrm{d}x = \int_{\mathbb{R}^3} |\chi_R\,u|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} |\xi_R\,u|^2\,\mathrm{d}x$$
$$\text{and} \quad \int_{\mathbb{R}^3} V\,|u|^2\,\mathrm{d}x = \int_{\mathbb{R}^3} V\,|\chi_R\,u|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} V\,|\xi_R\,u|^2\,\mathrm{d}x\,,$$

and the IMS truncation identity (see e.g. [27, 38]):

$$\int_{\mathbb{R}^3} |\nabla(\chi_R\,u)|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} |\nabla(\xi_R\,u)|^2\,\mathrm{d}x$$
$$= \int_{\mathbb{R}^3} |\nabla u|^2\,\mathrm{d}x - \int_{\mathbb{R}^3} |u|^2\,\underbrace{(\chi_R\Delta\chi_R + \xi_R\Delta\xi_R)}_{=O(R^{-2})\text{ as }R\to\infty}\,\mathrm{d}x\,. \tag{12}$$

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:*

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

as $R \to +\infty$.

Proof. The assertion for $\mathcal{E}_{\mathrm{kin}}[\rho]$ is a straightforward consequence of (12), namely

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

For the entropy term, we can use the *Brown-Kosaki inequality* (cf. [3]) as in [8, Lemma 3.4] to obtain

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

□

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 (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 $\tau_y : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ 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* (7) *and assume that (β1)–(β2) 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*

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

(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*

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

As a consequence, $T^*>0$ *and* $T^*(M)=+\infty$ *for any* $M>0$ *if* $\lim_{s\to0_+}\beta(s)/s^3=0$.

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 $\mathcal{F}_T[\rho]\le i_{M-m,T}+\varepsilon$ and $\mathcal{F}_T[\sigma]\le i_{m,T}+\varepsilon$. 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 $B(0,R)$ of $\mathbb{R}^3$, for some $J\in\mathbb{N}$. After approximating σ analogously, we define $\sigma_{R\mathsf{e}}:=\tau^*_{3R\mathsf{e}}\,\sigma\,\tau_{3R\mathsf{e}}$, where $\mathsf{e}\in\mathbb{S}^2\subset\mathbb{R}^3$ is a fixed unit vector and τ is the translation operator defined above. Note that we have $\rho\,\sigma_{R\mathsf{e}}=\sigma_{R\mathsf{e}}\,\rho=0$, hence $\rho+\sigma_{R\mathsf{e}}\in\mathfrak{H}_M$ and $\operatorname{tr}\beta(\rho+\sigma_{R\mathsf{e}})=\operatorname{tr}\beta(\rho)+\operatorname{tr}\beta(\sigma_{R\mathsf{e}})$. Thus we have

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

where the $O(1/R)$ term has in fact negative sign so that we can simply drop it. Taking the limit $\varepsilon\to0$ yields the desired inequality.

Next, consider a minimizer ρ of $\mathcal{E}_H$ subject to $\operatorname{tr}\rho=M$. It is given by an appropriate rescaling of the pure state obtained in [16]. 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 λ, the Hartree energy $\mathcal{E}_H[\rho_\lambda]=\lambda^2\,\mathcal{E}_{\rm kin}[\rho]-\lambda\,\mathcal{E}_{\rm pot}[\rho]$ has a minimum for some $\lambda>0$. Computing $\frac{\rm d}{{\rm d}\lambda}\,\mathcal{E}_H[\rho_\lambda]=0$, we infer that $\lambda=\mathcal{E}_{\rm pot}[\rho]/(2\,\mathcal{E}_{\rm kin}[\rho])$ and moreover

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

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

$$\mathcal{F}_T[\rho]=i_{M,0}+T\,\beta(M)=\beta(M)\,\left(T-\frac{M^3}{\beta(M)}|i_{1,0}|\right)\ge i_{M,T}\;,\tag{13}$$

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

Since β 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

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

By the sub-additivity inequality and (13), we obtain

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

for any $n \in \mathbb{N}^*$. Since $\lim_{s\to 0_+} \beta(s)/s = 0$, we find that $i_{M,T} \leq 0$ by passing to the limit as $n \to \infty$. In the particular case $\lim_{s\to 0_+} \beta(s)/s^3 = 0$, we conclude that $T^*(M) = +\infty$ for any $M > 0$. Similarly, using again the sub-additivity inequality and (13), 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 $T^* < \infty$. □

2.3. Euler-Lagrange equations and Lagrange multipliers

As in [10, 8], 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 (β1)–(β2) hold. Consider a density matrix operator $\rho \in \mathfrak{H}_M$ which minimizes $\mathcal{F}_T$. Then ρ is such that*

$$\mathrm{tr}(V_\rho\,\rho) = 4\,\mathrm{tr}(-\Delta\,\rho) \tag{14}$$

and satisfies the self-consistent equation

$$\rho = (\beta')^{-1}\big((\mu - H_\rho)/T\big)\,, \tag{15}$$

where H_ρ is the mean-field Hamiltonian defined in (5) *and $\mu \leq 0$ denotes the Lagrange multiplier associated to the mass constraint* $\mathrm{tr}\,\rho = M$. *Explicitly, μ is given by*

$$\mu = \frac{1}{M}\,\mathrm{tr}\left(\left(H_\rho + T\,\beta'(\rho)\right)\rho\right)\,. \tag{16}$$

Proof. Let $\rho \in \mathfrak{M}_M$ be a minimizer of $\mathcal{F}_T$. Consider the decomposition given by (1). If we denote by ρ_λ 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 $\mathcal{E}_H[\rho_\lambda] = \lambda^2\,\mathcal{E}_{\mathrm{kin}}[\rho] - \lambda\,\mathcal{E}_{\mathrm{pot}}[\rho]$ while $\mathcal{S}[\rho_\lambda] = \mathcal{S}[\rho]$ for any $\lambda > 0$. Hence the condition $\frac{d\mathcal{E}_H[\rho_\lambda]}{d\lambda}_{|\lambda=1} =$

0 exactly amounts to $\mathcal{E}_{\rm pot}[\rho] = 2\,\mathcal{E}_{\rm kin}[\rho]$. 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 ρ also solves the linearized problem

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

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

Clearly, ρ given by (15) is a stationary solution to the time-dependent Hartree system (4), since ρ is a function of the Hamiltonian H_ρ. In order to get more insight, we can use the decomposition (1) to rewrite the stationary Hartree model in terms of (at most) countably many eigenvalue problems coupled through a nonlinear Poisson equation

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

where $(\mu_j)_{j\in\mathbb{N}} \in \mathbb{R}$ denotes the sequence of the eigenvalues of H_ρ and

$$\langle \psi_j, \psi_k \rangle_{L^2} = \delta_{j,k}\ .$$

The self-consistent equation (15) consequently implies the following relation between the occupation numbers $(\lambda_j)_{j\in\mathbb{N}}$ and the eigenvalues $(\mu_j)_{j\in\mathbb{N}}$:

$$\lambda_j = (\beta')^{-1}((\mu - \mu_j)/T)_+\ , \tag{17}$$

where $s_+ = (s + |s|)/2$ denotes the positive part of s. Upon reverting the relation (17) we obtain $\mu_j = \mu - T\,\beta'(\lambda_j)$ for any $\mu_j \le \mu$.

The Lagrange multiplier μ 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

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

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

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 μ be the corresponding Lagrange multiplier. With the above notations, if $p(M) \le 3$, then $M\,\mu \le p(M)\, i_{M,T} < 0$.*

Proof. By definition of $i_{M,T}$ and according to (16), we know that

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

Using (14), 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. □

The negativity of the Lagrange multiplier μ, is straightforward in the zero temperature case. In our situation it holds under Assumption (β3), 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 ρ, monotonicity easily follows. □

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. [15]. 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,*

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

This result is the analog of [15, 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 $\rho \in \mathfrak{H}_M$,*

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

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

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

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

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

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 $\|n_\rho\|_{L^3}$:

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

We conclude as in (10) using Sobolev's inequality to control $\|n_\rho\|_{L^3}$ by $\mathrm{tr}(-\Delta\,\rho)$. □

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 χ_R be the cut-off function given in (11). By Lemma 2.2 we have

$$\mathrm{tr}(-\Delta\,(\chi_R\,\rho^{(\ell)}\,\chi_R)) \le \mathrm{tr}(-\Delta\,\rho^{(\ell)}) + O(R^{-2}) \qquad \text{and} \quad \mathrm{tr}\,\beta(\chi_R\,\rho^{(\ell)}\,\chi_R) \le \mathrm{tr}\,\beta(\rho^{(\ell)})\;.$$

To handle the potential energies, we observe that

$$\begin{aligned}\Big|\,\mathcal{E}_{\mathrm{pot}}[\chi_R\,\rho^{(\ell)}\,\chi_R] - \mathcal{E}_{\mathrm{pot}}[\rho^{(\ell)}]\,\Big| &\le \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{(1-\chi_R^2(x)\,\chi_R^2(y))\,n_{\rho^{(\ell)}}(x)\,n_{\rho^{(\ell)}}(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y \\ &\le \iint_{\{|x|\ge R\}\times\{|y|\ge R\}} \frac{n_{\rho^{(\ell)}}(x)\,n_{\rho^{(\ell)}}(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y\;.\end{aligned}$$

Using Lemma 3.1 and Lemma 3.2, we obtain

$$\Big|\,\mathcal{E}_{\mathrm{pot}}[\chi_R\,\rho^{(\ell)}\,\chi_R] - \mathcal{E}_{\mathrm{pot}}[\rho^{(\ell)}]\,\Big| \le C\,\Big[\mathrm{tr}(-\Delta\,\rho^{(\ell)})\Big]^{1/2} \int_{|x|\ge R} n_{\rho^{(\ell)}}(x)\,\mathrm{d}x \le O(R^{-2})$$

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

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

Consider now the test state

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

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

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

for some positive constant C, which yields the desired result for R sufficiently large. □

4. Existence of minimizers below T^*

By a classical result, see e.g. [15, 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 $n_{\rho_k}\to n_\rho$ almost everywhere as $k\to\infty$. Then $\rho_k\to\rho$ strongly in $\mathfrak{H}$ if and only if* $\operatorname{tr}\rho=M$.

Proof. The proof relies on a characterization of the compactness due to Brezis and Lieb (see [2] and [17, Theorem 1.9]) from which it follows that

$$\begin{aligned}\lim_{k\to\infty}\left(\int_{\mathbb{R}^3}n_{\rho_k}\,\mathrm{d}x-\int_{\mathbb{R}^3}|n_\rho-n_{\rho_k}|\,\mathrm{d}x\right)=\int_{\mathbb{R}^3}n_\rho\,\mathrm{d}x\\ \text{and}\quad\lim_{k\to\infty}\Big(\operatorname{tr}(-\Delta\,\rho)-\operatorname{tr}\big(-\Delta\,(\rho-\rho_k)\big)\Big)=\operatorname{tr}(-\Delta\,\rho)\,.\end{aligned}$$

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 $\lim_{k\to\infty}\operatorname{tr}(-\Delta\,(\rho-\rho_k))=0$ if and only if $\operatorname{tr}\rho=M$. □

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 $n\to\infty$, 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. [20]. 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 (β1)–(β3) hold. Let* $M > 0$ *and consider* $T^* = T^*(M)$ *defined by* (8). *For all* $T < T^*$, *there exists an operator* ρ *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 [15]. Compared to previous results (see for instance [22, 23, 24, 15]), the main difficulty arises in the splitting case, as we shall see below.

Step 1: Non-vanishing. We split

$$\mathcal{E}_{\rm pot}[\rho_n] = \iint_{\mathbb{R}^6} \frac{n_{\rho_n}(x)\, n_{\rho_n}(y)}{|x-y|}\, \mathrm{d}x\, \mathrm{d}y$$

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_{ρ_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

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

and directly get bounds on I_2 and I_3 by computing

$$I_2 \le R \iint_{|x-y|<R} n_{\rho_n}(x)\, n_{\rho_n}(y)\, \mathrm{d}x\, \mathrm{d}y \le R\, M \sup_{y\in\mathbb{R}^3} \int_{y+B_R} n_{\rho_n}(x)\, \mathrm{d}x\ ,$$
$$I_3 \le \frac{1}{R} \iint_{\mathbb{R}^6} n_{\rho_n}(x)\, n_{\rho_n}(y)\, \mathrm{d}x\, \mathrm{d}y \le \frac{M^2}{R}\ .$$

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

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

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

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

for R big enough and for some sequence $(a_n)_{n\in\mathbb{N}}$ of points in $\mathbb{R}^3$. Replacing ρ_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 $M^{(1)} = \int_{\mathbb{R}^3} n_{\rho^{(1)}}\, \mathrm{d}x > 0$.

Step 2: Dichotomy. Either $M^{(1)} = M$ and ρ_n strongly converges to ρ in $\mathfrak{H}$ by Lemma 4.1, or $M^{(1)} \in (0, M)$. Let us choose R_n such that $\int_{\mathbb{R}^3} n_{\rho_n^{(1)}}\, \mathrm{d}x = M^{(1)} + (M - M^{(1)})/n$ 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, $\lim_{n\to\infty} R_n = \infty$. By Step 1, we know that $\rho_n^{(1)}$ strongly converges to $\rho^{(1)}$. By Identity (12) and Lemma 2.2, we find that

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

thus showing that

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

By step 1, $\lim_{n\to\infty} \int_{\mathbb{R}^3} n_{\rho_n^{(2)}}\, \mathrm{d}x = M - M^{(1)}$. By sub-additivity, according to Proposition 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 $i_{M,T} = i_{M^{(1)},T}$, 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. □

As a direct consequence of the variational approach, the set of minimizers $\mathfrak{M}_M$ is *orbitally stable* under the dynamics of (4). To this end, we note that global in-time existence of solutions $\rho(t) \in \mathfrak{H}$ follows from the arguments given in [6, 29] (see also [1], where a slightly more general class of equations is studied). To quantify the stability, define

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

Corollary 4.3. *Assume that (β1)–(β3) hold. For any given $M > 0$, let $T \in (0, T^*(M))$. For any $\varepsilon > 0$, there exists $\delta > 0$ such that, for all $\rho_{\mathrm{in}} \in \mathfrak{H}_M$ with $\mathrm{dist}_{\mathfrak{M}_M}(\rho_{\mathrm{in}}) \leq \delta$,*

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

where $\rho(t)$ is the solution of (4) *with initial data $\rho_{\mathrm{in}} \in \mathfrak{H}_M$.*

Similar results have been established in many earlier papers like, for instance in [26] in the case of repulsive Coulomb interactions. As in [5, 26], 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 [16], 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 ρ_{T_0} the minimizer for $\mathcal{F}_{T_0}$, we obtain

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

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. □

Consider T_c defined by (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 [16] 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

$$H_0 := -\Delta - |\psi_0|^2 * |\cdot|^{-1} = H_{\rho_0} \tag{18}$$

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 (β1)–(β3) hold. With T_c defined by* (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 $\lim_{\to\infty} T_n = 0$. 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 (17), we know that

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

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

$$\lim_{n\to\infty} \mu_j^{(n)} = \mu_j^0 \le 0$$

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

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

By (17) and the fact that β' is increasing, this implies: $\mu^{(n)} > \mu_1^{(n)} \to \mu_1^0$ as $n \to \infty$. Then

$$M = \lambda_0^0 \ge \lim_{\to\infty} \lambda_0^{(n)} = \lim_{\to\infty} (\beta')^{-1}\left(\tfrac{\mu^{(n)} - \mu_0^{(n)}}{T_n}\right) \ge \lim_{\to\infty} (\beta')^{-1}\left(\tfrac{\mu_1^0 - \mu_0^{(n)}}{T_n}\right) = +\infty\,.$$

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 [16], we know that it is unique and given by ρ_0, in which case $i_{M,T} = i_{M,0} - T\,\mathcal{S}[\rho_0] = i_{M,0} + T\,\beta[M]$. □

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

Corollary 5.3. *Assume that (β1)–(β3) 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 $T > T_c$. □

We finally give a characterization of T_c.

Proposition 5.4. *Assume that (β1)–(β3) hold. For any $M > 0$, the critical temperature satisfies*

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

where μ_0^0 and μ_1^0 are the two lowest eigenvalues of H_0 defined in (18).

Proof. For $T \le T_c$, there exists a unique pure state minimizer ρ_0. For such a pure state, the Lagrange multiplier associated to the mass constraint $\operatorname{tr}\rho_0 = M$ is given by $\mu = \mu(T)$. According to (16), 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 $0 \ne \lambda_1 = (\beta')^{-1}\big((\mu_1^0 - \mu(T))/T\big)$ if $T > (\mu_1^0 - \mu_0^0)/\beta'(M)$, thus proving that $T_c \le (\mu_1^0 - \mu_0^0)/\beta'(M)$.

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 ρ be a minimizer for $T = T_c$. The two inequalities, $i_{M,0} \le \mathcal{E}_H[\rho]$ and $\beta(M) \le \operatorname{tr}\beta(\rho)$ hold as equalities if and only if, in both cases, ρ is of rank one. Consider a sequence $(T^{(n)})_{n\in\mathbb{N}}$ such that $\lim_{n\to\infty} T^{(n)} = T_c$, $T^{(n)} > T_c$ for any $n \in \mathbb{N}$ and, if $(\rho^{(n)})_{n\in\mathbb{N}}$ denotes a sequence of associated minimizers with $\big(\mu_j^{(n)}\big)_{j\in\mathbb{N}}$ and $\mu^{(n)} \le 0$ 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 $\lim_{n\to\infty} \lambda_1^{(n)} = 0$, so that $\lim_{n\to\infty} \mu^{(n)} = \mu_1^0$. 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. □

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 [9], we know that

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

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

$$\sum_j |\mu_j(V)|^\gamma \leq C_{\mathrm{LT}}(\gamma)\int_{\mathbb{R}^3} |V|^q\,\mathrm{d}x$$

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

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

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

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

Next, we invoke the Hardy-Littlewood-Sobolev inequality

$$\int_{\mathbb{R}^3} |V_\rho|^q\,\mathrm{d}x \leq C_{\mathrm{HLS}}\,\|n_\rho\|^q_{L^r(\mathbb{R}^3)}$$

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

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

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

$$\int_{\mathbb{R}^3} |V_\rho|^q\,\mathrm{d}x \leq c\,M^{q\,\theta}\,\left(\mathrm{tr}(-\Delta\,\rho)\right)^{q\,(1-\theta)}$$

for some positive constant c and, as a consequence,

$$\mathcal{F}_T[\rho] \geq \frac{1}{2}\,\mathrm{tr}(-\Delta\,\rho) - T^{-\frac{1}{p-1}}\,\mathsf{K}\,\mathrm{tr}(-\Delta\,\rho)^{q\,(1-\theta)}, \tag{19}$$

for some $\mathsf{K} > 0$. Moreover we find that

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

so that η 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 $\operatorname{tr}\beta(\rho)$ is positive, as in the proof of (10), we know that for some positive constant C, which is independent of $T > 0$,

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

and, as a consequence,

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

On the other hand, by (19), we know that $\mathcal{F}_T[\rho] < 0$ means that

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

The compatibility of these two conditions amounts to

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

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* $\lim_{T\to T^*_-} i_{M,T} = 0$.

Proof. The proof follows from the concavity of $T \mapsto i_{M,T}$ (see Lemma 5.1). Let ρ_{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 (8) if $\liminf_{T\to T^*_-} i_{M,T} < 0$. □

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*

$$M\,\frac{\partial\, i_{M,T}}{\partial M} + (3-p)\,T\,\frac{\partial\, i_{M,T}}{\partial T} \leq 3\,i_{M,T} \tag{20}$$

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), define

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

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

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

which proves (20) by differentiating at $\lambda = 1$. In case (i), since $T \mapsto i_{M,T}$ is non-decreasing, we have

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

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

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

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

Assume that $\beta(s) = s^p$ for any $s \in \mathbb{R}^+$. We observe that for $T < T^*(M)$, $\frac{\partial\, i_{M,T}}{\partial M} \le \frac{3}{M}\, i_{M,T}$ if $p \le 3$, 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 β satisfying Assumptions (β1) and (β2) 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 β, 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 ρ of Proposition 3.1 and let $\mu < 0$ be the Lagrange multiplier corresponding to the mass constraint $\operatorname{tr}\rho = M$. Define

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

The density operator ρ 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 ρ also solves the linearized minimization problem $\inf_{\sigma\in\mathfrak{H}} \mathcal{L}^\mu[\sigma]$ where

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

Consider the cut-off functions χ_R and ξ_R defined in (11) and let $\rho_R := \chi_R\,\rho\,\chi_R$. By Lemma 2.2, we know that, as $R \to \infty$,

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

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

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

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

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

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

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

In summary this yields

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

Collecting all estimates, we have proved that

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

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

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

for R large enough, which completes the proof of Proposition 3.1. □

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