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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.

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 ρ can be decomposed as

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

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

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

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

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

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

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

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

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

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

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

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 $\mathscr{F}_T$ 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

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

Here $[A,B] = AB - BA$ 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 [5]) 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 [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 (4) or, equivalently, (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 $\mathscr{F}_T[\rho]$ reduces to the gravitational Hartree energy $\mathscr{E}_H[\rho]$. 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 $\mathscr{F}_T[\rho]$ 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 $\mathscr{F}_T$, 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 $\mathscr{F}_T$ 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. [16, 11, 13]. Moreover, depending on the choice of β, it could happen that $T^* = +\infty$, in which case minimizers of $\mathscr{F}_T$ 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 $\mathscr{F}_T$, defined in (3), by

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

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. [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

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

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 $\mathscr{F}_T[\rho] = i_{M,T}$. 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) *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 $T \to T^* < +\infty$. 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 $\mathscr{F}_T$ introduced in (3) is well defined and $i_{M,T} > -\infty$.

Lemma 2.1. *Assume that (β1)–(β2) hold. The free energy $\mathscr{F}_T$ is well-defined on $\mathfrak{H}_M$ and $i_{M,T}$ is bounded from below. If $\mathscr{F}_T[\rho]$ 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 $\mathscr{E}_{\mathrm{pot}}[\rho]$ can be bounded in terms of the kinetic energy. To this end, note that for every $\rho \in \mathfrak{H}$ we have

$$\mathscr{E}_{\mathrm{pot}}[\rho] \le C\,\|n_\rho\|_{L^1}^{3/2}\,\|n_\rho\|_{L^3}^{1/2}$$

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), is bounded by $\mathrm{tr}(-\Delta\rho)$. Hence we can conclude that

$$\mathscr{E}_{\mathrm{pot}}[\rho] \le C\,\|n_\rho\|_{L^1}^{3/2}\,\mathrm{tr}(-\Delta\rho)^{1/2} \tag{10}$$

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

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

uniformly w.r.t. $\rho \in \mathscr{H}_M$, thus establishing a lower bound on $i_{M,T}$. For the entropy term $\mathscr{S}[\rho] = -\mathrm{tr}\,\beta(\rho)$ we observe that, since β is convex and $\beta(0) = 0$, it holds $0 \le \beta(\rho) \le \beta(M)\,\rho$ 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 $\mathscr{F}_T$ 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 $|x| \ge 2$. 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

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

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:*

$$\mathscr{S}[\rho_R^{(1)}] + \mathscr{S}[\rho_R^{(2)}] \ge \mathscr{S}[\rho] \quad \textit{and} \quad \mathscr{E}_{\mathrm{kin}}[\rho_R^{(1)}] + \mathscr{E}_{\mathrm{kin}}[\rho_R^{(2)}] \le \mathscr{E}_{\mathrm{kin}}[\rho] + O(R^{-2})$$

as $R \to +\infty$.

Proof. The assertion for $\mathscr{E}_{\mathrm{kin}}[\rho]$ 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. [2]) as in [6, Lemma 3.4] to obtain

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

□

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*

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

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

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

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

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

Next, consider a minimizer ρ of $\mathscr{E}_H$ subject to $\operatorname{tr} \rho = M$. 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 λ, the Hartree energy $\mathscr{E}_H[\rho_\lambda] = \lambda^2 \, \mathscr{E}_{\mathrm{kin}}[\rho] - \lambda \, \mathscr{E}_{\mathrm{pot}}[\rho]$ has a minimum for some $\lambda > 0$. Computing $\frac{\mathrm{d}}{\mathrm{d}\lambda} \mathscr{E}_H[\rho_\lambda] = 0$, we infer that $\lambda = \mathscr{E}_{\mathrm{pot}}[\rho] / (2\,\mathscr{E}_{\mathrm{kin}}[\rho])$ and moreover

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

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

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

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

Since β is non-negative function on $[0, \infty)$, the map $T \mapsto \mathscr{F}_T[\rho]$ 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

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

for any $n \in \mathbb{N}^*$. Since $\lim_{s\to 0_+} \beta(s)/s = 0$, we find that $i_{M,T} \le 0$ 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

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

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 $i_{M,T} \le i_{M,T_0} + (T - T_0)\,\beta(M)$ 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 (β1)–(β2) hold. Consider a density matrix operator $\rho \in \mathfrak{H}_M$ which minimizes $\mathscr{F}_T$. 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 $\mu \le 0$ denotes the Lagrange multiplier associated to the mass constraint* $\mathrm{tr}\,\rho = M$*. Explicitly, μ is given by*

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

Proof. Let $\rho \in \mathfrak{M}_M$ be a minimizer of $\mathscr{F}_T$. 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 $\mathscr{E}_H[\rho_\lambda] = \lambda^2\,\mathscr{E}_{\rm kin}[\rho] - \lambda\,\mathscr{E}_{\rm pot}[\rho]$ while $\mathscr{S}[\rho_\lambda] = \mathscr{S}[\rho]$ for any $\lambda > 0$. Hence the condition $\frac{d}{d\lambda}\mathscr{E}_H[\rho_\lambda]_{|\lambda=1} = 0$ exactly amounts to $\mathscr{E}_{\rm pot}[\rho] = 2\,\mathscr{E}_{\rm kin}[\rho]$. Next, let $\sigma \in \mathfrak{H}_M$. Then $(1-t)\,\rho + t\,\sigma \in \mathfrak{H}_M$ and

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

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

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

Computing the corresponding Euler-Lagrange equations shows that the minimizer of this problem is $\rho = (\beta')^{-1}\left((\mu - H_\rho)/T\right)$ where μ denotes the Lagrange multiplier associated to the constraint $\operatorname{tr}\rho = M$. 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 $(0,\infty)$. □

Using the decomposition (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_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 $(\mu_j)_{j\in\mathbb{N}}$:

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

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

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

Notice that if (β3) 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 $\mathscr{F}_T$ 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

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

Using (14), we end up with the identity

$$p(M)\,i_{M,T} - M\,\mu = (3-p(M))\,\operatorname{tr}(-\Delta\rho) + T\,\operatorname{tr}\left(p(M)\,\beta(\rho) - \beta'(\rho)\,\rho\right) \ge 0\,,$$

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

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

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. $\square$

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

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

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* subadditivity 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 $\mathscr{F}_T$. 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 [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 $\rho \in \mathfrak{H}_M$,*

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

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

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

To handle the potential energies, we observe that

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

Using Lemma 3.1 and Lemma 3.2, we obtain

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

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

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

Consider now the test state

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

for some unit vector $\mathrm{e}\in\mathbb{S}^2$. 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

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

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

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 $\mathscr{F}_T$, 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 [1] and [15, Theorem 1.9]) from which it follows that

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

By semi-continuity of $\mathscr{F}_T$, monotonicity of $M\mapsto i_{M,T}$ according to Proposition 2.3 (ii) and compactness of the quadratic term in $\mathscr{E}_H$, 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 $\mathscr{F}_T$. To this end, consider a minimizing sequence $(\rho_n)_{n\in\mathbb{N}}$ for $\mathscr{F}_T$ 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. [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 (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 $\mathscr{F}_T[\rho] = i_{M,T}$. 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

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

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

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

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

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

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

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

for R big enough and for some sequence $(a_n)_{n\in\mathbb{N}}$ of points in $\mathbb{R}^3$. Replacing 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

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

thus showing that

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

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 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. □

As a direct consequence of the variational approach, the set of minimizers $\mathfrak{M}_M$ is *orbitally stable* under the dynamics of (4). To quantify this 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 [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

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

Denoting by ρ_{T_0} the minimizer for $\mathscr{F}_{T_0}$, we obtain

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

which means that $|\mathscr{S}[\rho_{T_0}]|$ 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 [14] proved that $\mathscr{F}_{T=0} = \mathscr{E}_H$ 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

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

where, for any $n \in \mathbb{N}$, $\left(\mu_j^{(n)}\right)_{j\in\mathbb{N}}$ 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 $\mathscr{F}_{T=0}$, we know that

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

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

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

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

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

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 $\mathscr{F}_T$ in $\mathfrak{H}_M$ is also a minimizer of $\mathscr{E}_H + T\,\beta(M)$. From [14], we know that it is unique and given by ρ_0, in which case $i_{M,T} = i_{M,0} - T\,\mathscr{S}[\rho_0] = i_{M,0} + T\,\beta[M]$. ☐

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 $T \leq T_c$, 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 $0 \neq \lambda_1 = (\beta')^{-1}\big((\mu_1^0 - \mu(T))/T\big)$ if $T > (\mu_1^0 - \mu_0^0)/\beta'(M)$, thus proving that $T_c \leq (\mu_1^0 - \mu_0^0)/\beta'(M)$.

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 ρ be a minimizer for $T = T_c$. The two inequalities, $i_{M,0} \leq \mathscr{E}_H[\rho]$ and $\beta(M) \leq \operatorname{tr}\beta(\rho)$ 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 $\mu^{(n)} \leq 0$ 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 $\lim_{n\to\infty} \lambda_1^{(n)} = 0$, 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 [7], we know that

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

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

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

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

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

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

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

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 $\operatorname{tr}(-\Delta\rho)$, we conclude that

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

for some positive constant c and, as a consequence,

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

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

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

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 $\mathscr{F}_T[\rho] = i_{M,T}$. Since $\mathrm{tr}\,\beta(\rho)$ is positive, as in the proof of (10), we know that for some positive constant C, which is independent of $T > 0$,

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

and, as a consequence,

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

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

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

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 $\mathscr{F}_T[\rho]$.

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 $\mathscr{F}_{T_0}[\rho_{T_0}] = -\delta$ for some $\delta > 0$. Then we observe

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

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 (β3) 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 $p \le 3$. 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*

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

and, as a consequence:

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

(ii) if $p \ge 3$, then $i_{M,T} \le (\frac{T}{T_0})^{3/(3-p)}\, i_{M,T_0}$ 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 $M[\rho] := \operatorname{tr} \rho = \int_{\mathbb{R}^3} n_\rho \,\mathrm{d}x$, we find that

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

and

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

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 $\lambda = (T/T_0)^{1/(3-p)}$. $\square$

Assume that $\beta(s) = s^p$ for any $s \in \mathbb{R}^+$. We observe that for $T < T^*(M)$, $\frac{\partial i_{M,T}}{\partial M} \le \frac{3}{M} i_{M,T}$ 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.

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

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

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

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

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 $R \to \infty$,

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

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

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

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

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

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

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

Collecting all estimates, we have proved that

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

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

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