Dissertation

Analysis of Hartree systems: semi-classical asymptotics and themal effects for ground states

zur Erlangung des akademischen Grades

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Abstract

This thesis consists of two independent parts. The first part, treated in Chapters 2 and 3, deals with the asymptotics of semi-relativistic Schrödinger equations in the semi-classical regime. To this end, we first study, in Chapter 2, a free evolution equation as a simple motivating model. We aim to describe the asymptotics of the highly oscillating solutions propagated by the semi-relativistic Schrödinger operator. We employ the method of stationary phase - which can be regarded as a generalization of WKB methods - to deal with such kind of oscillations in their asymptotic description.

Then the third chapter is devoted to the classical limit of the three-dimensional semi-relativistic Hartree model for fast quantum mechanical particles moving in a self-consistent field. We give new interpolation estimates (Lieb-Thirring type inequalities) to obtain uniform bounds in terms of the relativistic energy. The main result of the third chapter is given in Section 4: Under appropriate assumptions on the initial density matrix as a (fully) mixed quantum state we prove, using Wigner transformation techniques, that its classical limit yields the well known relativistic Vlasov-Poisson system. The result holds for the case of attractive and repulsive mean-field interaction, with an additional size constraint on the initial data in the attractive case.

In part two, we consider the non-relativistic Hartree model with temperature and attractive Coulomb interactions. We prove that steady states of the system are achieved as the minimizers of a free energy functional under a mass constraint provided that the temperature of the system is below a certain threshold. The maximal temperature (or a limit mass, equivalently) arises as a result of the competition between the Hartree energy and the entropy term involved in the free energy. We also investigate whether those ground states are mixed or pure states and characterize a critical temperature above which mixed states appear.

Kurzfassung

Die vorliegende Arbeit besteht aus zwei unabhängigen Teilen. Der erste Teil, der die Kapitel 2 und 3 beinhaltet, beschäftigt sich mit der Asymptotik von semi-relativistischen Schrödinger-Gleichungen im semi-klassischen Regime. Zu Beginn, in Kapitel 2, analysieren wir eine freie Evolutionsgleichung als einfaches Motivationsmodell. Unser Ziel ist es, die Asymptotik von stark oszillierenden Lösungen, die durch den semi-relativistischen Schrödinger-Operator fortbewegt werden, zu beschreiben. Für eine asymptotische Beschreibung dieser Art von Oszillationen verwenden wir die Methode der stationären Phase, die als Verallgemeinerung der WKB-Methoden betrachtet werden kann.

Im dritten Kapitel beschäftigen wir uns mit dem klassischen Limes des dreidimensionalen semi-relativistischen Hartree-Modells für schnelle quantenmechanische Teilchen, die sich in einem selbstkonsistenten Feld bewegen. Neue Interpolationsabschätzungen (von Lieb-Thirring Art) führen zu gleichmäßigen Schranken bezüglich der relativistischen Energie. Das Hauptresultat von Kapitel 3 wird in Abschnitt 4 angeführt: Unter geeigneten Annahmen an die anfängliche Dichtematrix als (vollständig) gemischter Quantenzustand beweisen wir unter der Verwendung der Wigner-Transformation, dass der klassische Limes zum wohlbekannten relativistischen Vlasov-Poisson System führt. Dieses Ergebnis gilt sowohl für anziehende als auch für abstoßende Mean-Field Wechselwirkungen, mit einer zusätzlichen Einschränkung für die Größe der Anfangsdaten im anziehenden Fall.

Im zweiten Teil betrachten wir das nicht-relativistische Hartree-Modell mit Temperatur- und anziehenden Coulomb-Wechselwirkungen. Wir zeigen, dass stationäre Zustände des Systems durch Minimierung des freien Energie-Funktionals unter einer Bedingung an die Masse erreicht werden, vorausgesetzt, dass sich die Temperatur des Systems unterhalb eines gewissen Grenzwertes befindet. Die maximale Temperatur (oder, äquivalent dazu, eine Grenzmasse) enstehen durch die Konkurrenz der Hartree-Energie und des Entropieterms involviert in der freien Energie. Wir untersuchen weiters, ob diese Grundzustände von gemischtem oder reinem Typ sind und beschreiben eine kritische Temperatur, über welcher gemischte Zustände auftreten.

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Contents

Chapter 1

Introduction

This thesis deals with the mathematical analysis of mean-field equations, involving self-consistent potentials of Hartree type. Such models are known (see, e.g., [2, 3, 4, 5, 6]) to provide a valuable description of many body quantum system. To this end, the state of a quantum system is represented by a *wavefunction*, or more generally (in the case of statistically mixed states) by a *density matrix operator*. The dynamics of the system is described by Schrödinger type equations (including self-consistent potentials). In the first part of the thesis we consider *semi-relativistic* Schrödinger equations in the *semi-classical* regime. The non-local semi-relativistic operator is a scalar pseudo-differential operator, i.e. $\sqrt{-\Delta + 1}$, conveniently replacing the full (matrix-valued) Dirac operator which is compatible with special relativity.

Chapter 2 in Part I, is devoted to the simple model of a free evolving semi-relativistic particle in the semi-classical regime. This comprises a highly oscillatory problem, since the wave function oscillates with frequency $1/\varepsilon$, where ε is the small semi-classical parameter (i.e. the scaled Planck's constant). The analysis given in Chapter 2 is restricted to give an asymptotic description for the semi-classical scaled model in the sense of WKB-asymptotics, cf. [7]. The semi-classical regime refers to the situation in which the wavefunction of the system is approximately peaked around the solution of the corresponding classical equations of motion. Roughly speaking, the semi-classical regime can be regarded as a zoom out in time and space for a passage from quantum to classical theory. In leading order (or in the semi-classical limit) WKB-asymptotics give information on the evolution of the macroscopic quantities like the energy density, etc.

In this small chapter we consider an initial value problem for linear dispersive PDEs subject to highly oscillatory initial data. Since the oscillations (which propagate in the time) inhibit the solution from converging strongly in a suitable sense, the asymptotic description is by no means straightforward, in particular for physical observables in which we are interested. The traditional way to deal with this problem is introducing the WKB-ansatz. However, the non-local kinetic operator $\sqrt{-\Delta+1}$ does not allow the classical use of the WKB-ansatz (as it is done in the non-relativistic version). For that reason Chapter 2 focuses on *expanding the highly oscillating integral which represents the pseudo-relativistic operator* and then obtaining the lowest order equations corresponding to the phase-function and the amplitude which compose the wavefunction. In this sense the method of stationary phase can be regarded as a generalization of the WKB methods. The stationary phase method relies on the idea that locally the main contribution to the oscillating integral originates from the stationary points of the phase. This fact follows from the cancellation of sinusoids with rapidly varying phase.

In general (involving nonlinearities as well) WKB methods produce, in leading order, a Hamilton-Jacobi type equation for the phase and a conservation law for the energy density. These equations do not have global-in-time solutions, i.e., the system develops singularities in some finite time due to the characteristics of Hamilton-Jacobi equations. However, the use of *Wigner functions*, cf. [8], in the semi-classical limit of Schrödinger equations has been an alternative approach with increasing interest in recent decades. The real-valued Wigner transform of a quantum state describes the state of a particle ensemble in position-velocity phase space. Wigner functions are approved tools to deal with the semi-classical limits of observables.

The core part of Chapter 3 involves the semi-classical limit of the mean field dynamics of a self-interacting particle ensemble under consideration of relativistic effects, i.e., semi-relativistic Hartree systems (or semi-relativistic Schrödinger-Poisson system). Hartree systems emerge as a consequence of the coupling of the potential of the system with the density via the Poisson equation. The sign in front of the density eventually determines the attractive or repulsive nature of the system. We will present the mathematical setting of the model in the introduction of Chapter 3 as well as a brief description of the Wigner functions and their properties. Since the Wigner function is real-valued it can be seen as a quantum mechanical analogue of a classical phase space distribution. Hence, it satisfies a kinetic-like evolution equation. However, Wigner functions in general take negative values and do not allow for a probabilistic interpretation. Nevertheless, the Wigner transform of a semi-classical scaled quantum state has positive accumulation points in a suitable topology when this small parameter tends to zero such that the limiting measures can be identified as a distributional solution of the corresponding limiting evolutionary system. In our case it is shown to be a solution of the relativistic Vlasov-Poisson system.

The novelty of this study lies in the fact that new suitable interpolation estimates are needed to be established based on the relativistic kinetic energy in order to pass to the limit in the non-linear potential. To our knowledge, interpolation estimates (also referred to as Lieb-Thirring type inequalities) have been given only in the non-relativistic framework. Eventually, these type of estimates lead to (uniform) bounds in terms of the kinetic energy which are needed for compactness arguments in the limit procedure.

In Part II, Chapter 4, we discuss the ground states of attractive Hartree systems with temperature in non-relativistic framework. Throughout Chapter 4 we will mostly adopt the density matrix operator setting. The ground states of attractive Hartree systems, which are obtained as minimizers of Hartree energy under a mass constraint, are known to be pure states, i.e., rank one density matrices. Mixed states only appear as minimizers when the Hartree energy is modified by an entropy term with a temperature parameter in front. This additional term is also referred to as Casimir functionals (from classical mechanics), cf. [1] which are conserved quantities along the evolution, and in a quantum set-up they allow us to relate the eigenvalues of the Schrödinger operator with the occupation numbers. This approach also leads to an orbital (dynamical) stability result for steady states. Because of its interpretation in physics we call the energy-Casimir functional as *the free energy*.

For the minimization of the free energy we employ a variational approach under a mass constraint. Our existence analysis relies on the concentration-compactness method. This method allows us to deal with the lack of convexity due to the gravitational interaction among the particles which is the stellar dynamic case and in sharp contrast with the repulsive case, in turn, inducing weakly-lower-semicontinuous (free) energy functional. On the other hand, the competition between the Hartree energy and the entropy term gives rise to a *maximal temperature* or equivalently *maximal mass*. This has to be distinguished from the Chandrasekhar limit mass for white dwarfs which emerges in the semi-relativistic framework. We also identify the minimizers as a certain class of stationary solutions to the time-dependent Hartree system.

Apart from the existence of minimizers, we also introduce a *critical temperature* below which the ground state is a pure state and above which the ground state is a mixed state, if it exists. We shall prove that this critical temperature is positive, and always well-defined.

Each chapter is essentially self-contained with its own introduction in more detail and introduces its own notation according to its problem under consideration, although the main definitions throughout the thesis are consistent.

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Part I

Semi-classical asymptotics in semi-relativistic regime

Chapter 2

A generalized WKB-method for semi-relativistic Schrödinger equations

2.1 Introduction

Semi-relativistic equations have interesting applications in quantum theory, for instance, as an effective description of relativistic *white dwarfs* and *neutron stars*, see e.g. [1, 2, 3, 4, 5]. The aim of this chapter is to consider the simplest model in this framework and to give an asymptotic description for the model in the sense of WKB-asymptotics (Wentzel-Kramers-Brillouin, see [8]) in the semi-classical regime. Hence, we consider the free semi-relativistic Schrödinger equation

$$\varepsilon \partial_t \psi^\varepsilon + i \left(\sqrt{-\varepsilon^2 \Delta + 1} \right) \psi^\varepsilon = 0 \quad x \in \mathbb{R}^n, t \in \mathbb{R}_+ \tag{2.1.1}$$

where the small parameter ε (widely called the semi-classical parameter in the literature) is the dimensionless scaled Planck constant, and the wavefunction $\psi^\varepsilon = \psi^\varepsilon(x,t)$ is a complex-valued function. Here, semi-classical regime refers to the situation in which the wavefunction of the system is approximately peaked around the solution of the corresponding classical equations of motion. Roughly speaking, the semi-classical regime can be regarded as a zoom out in time and space for a passage from quantum to classical theory, e.g. $t \to \frac{t}{\varepsilon}, \quad x \to \frac{x}{\varepsilon}$. The action of the scalar pseudo-relativistic operator can be given as follows

$$\begin{aligned}
\sqrt{-\varepsilon^2 \Delta + 1}\, f(x) &= \int \sqrt{\varepsilon^2 |k|^2 + 1}\, \hat{f}(k) e^{ix\cdot k} \mathrm{d}k \\
&= \frac{1}{\varepsilon^n} \int \sqrt{|\xi|^2 + 1}\, \hat{f}(\xi/\varepsilon) e^{ix\cdot\xi/\varepsilon} \mathrm{d}\xi \\
&= \frac{1}{(2\pi\varepsilon)^n} \int\int \sqrt{|\xi|^2 + 1}\, f(y) e^{i(x-y)\cdot\xi/\varepsilon} \mathrm{d}y \mathrm{d}\xi
\end{aligned} \tag{2.1.2}$$

where we used the Fourier transform in the following form

$$\hat{f}(\xi/\varepsilon) = \frac{1}{(2\pi)^n} \int f(y) e^{-iy\cdot\xi/\varepsilon} \mathrm{d}y.$$

Unless the other way is indicated throughout this chapter all the integrals extend over $\mathbb{R}^n$.

In order to get an insight into the problem let us consider the plane-wave initial datum for the equation (2.1.1):

$$\psi^\varepsilon(x,0) = e^{ik\cdot x/\varepsilon}. \tag{2.1.3}$$

The solution to the initial value problem (2.1.1) – (2.1.3) is explicitly given by

$$\psi^\varepsilon(x,t) = e^{i(k\cdot x/\varepsilon - \sqrt{|k|^2+1}\ t/\varepsilon)} \tag{2.1.4}$$

and hence we observe that the equation (2.1.1) propagates oscillations with $O(\varepsilon)$-wavelength in space and time. This class of problems is called *highly oscillatory problems* and is of interest in itself. In the framework of this study we employ a technique called the stationary phase method to deal with this kind of oscillations in their asymptotic description.

For this purpose, we consider the Cauchy problem

$$\begin{aligned} \varepsilon\partial_t\psi^\varepsilon + i\left(\sqrt{-\varepsilon^2\Delta+1}\right)\psi^\varepsilon = 0 \quad x\in\mathbb{R}^n, t\in\mathbb{R}_+ \\ \psi^\varepsilon(x,0) = a_I(x)e^{i\phi_I(x)/\varepsilon}. \end{aligned} \tag{2.1.5}$$

Since the oscillations created inhibit the solution $\psi^\varepsilon(x,t)$ from converging strongly in a suitable sense the asymptotic description ($\varepsilon\to 0$) is by no means straightforward. The traditional way to deal with this problem is the WKB approach where one seeks an asymptotic description for the solution $\psi^\varepsilon(x,t)$ in the following form:

$$\psi^\varepsilon(x,t) \approx a(x,t)\exp\left(i\phi(x,t)/\varepsilon\right), \tag{2.1.6}$$

and assuming that the real-valued phase-function $\phi(x,t)$ and the real-valued amplitude $a(x,t)$ are sufficiently smooth for $x\in\mathbb{R}^n$ and $t\in\mathbb{R}_+$. As easily can be noted, even in formal level, plugging the *ansatz* (2.1.6) and obtaining the lowest order equations (as it is done in the non-relativistic case) is not possible due to the nonlocal kinetic operator. For that reason the scope of this work is restricted to obtain a rigorous expansion for the highly oscillating integral which represents the pseudo-relativistic operator and then obtaining the lowest order equations corresponding to the phase-function $\phi(x,t)$ and the amplitude $a(x,t)$. In this sense the method of stationary phase can be regarded as a generalization of the WKB methods. This method has been also used to obtain the multi-valued solutions to the linear non-relativistic Schrödinger equations regarding the superpositions of WKB-modes (or "rays" in geometric optics), see [6] and references therein.

The rest of the chapter is organized as follows: In the following section we introduce a rigorous expansion for the oscillatory integrals, then in Section 2.3 we expose the corresponding WKB-system as an asymptotic description. The detailed computation are given in the last section as an appendix.

2.2 Stationary phase method for oscillatory integrals

This section is devoted to an approximation for the oscillatory integral that has been obtained after plugging the WKB-ansatz (2.1.6) to the pseudo-differential operator (2.1.2):

$$\begin{aligned}\sqrt{-\varepsilon^2\Delta+1}\;\psi^\varepsilon(t,x) &\approx \frac{1}{(2\pi\varepsilon)^n}\int\int \sqrt{|\xi|^2+1}\;a(t,y)e^{i(\phi(t,y)-(y-x)\cdot\xi)/\varepsilon}\mathrm{d}\xi\mathrm{d}y\\ &= \frac{1}{(2\pi\varepsilon)^n}\int\int \sqrt{|\xi|^2+1}\;a(t,y+x)e^{i(\phi(t,y+x)-y\cdot\xi)/\varepsilon}\mathrm{d}\xi\mathrm{d}y.\end{aligned} \tag{2.2.1}$$

The idea of using the stationary phase method for the oscillatory integrals comes from the fact that locally the main contribution to the oscillating integral stems from the stationary points of the phase with respect to y and ξ, i.e. the points $y = 0$ and $\xi = \nabla_y\phi$. This fact follows from the simple observation of the cancellation of sinusoids with rapidly-varying phase. Thus, the following theorem from [7] (Ch. 7, Theorem 7.7.7) gives the exact statement of the method:

Theorem 1. *Let ϕ be a real valued function in $\mathcal{C}^\infty(\mathbb{R}^{n+m})$. If K is a compact subset of $\mathbb{R}^{2n+m}$ and $f \in \mathcal{C}_0^\infty(K)$, $k \geq n$, then*

$$\begin{aligned}&\Bigg|\int\int f(y,\xi,x)e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon}\mathrm{d}y\mathrm{d}\xi\\ &\qquad -e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n\sum_{\nu=0}^{k-n}\frac{1}{\nu!} < i\varepsilon D_y, D_\xi >^\nu \left(e^{ir_x(y)/\varepsilon}f(y,\xi,x)\right)_{y=0,\ \xi=\nabla_y\phi(x)}\Bigg|\\ &\leq C\varepsilon^{(k+n)/2}\sum_{|\alpha|\leq 2k}\sup_{y,\xi} \mid D^\alpha_{y,\xi}f(y,\xi,x)\mid .\end{aligned}$$

Here $r_x(y) = \phi(y+x) - \phi(x) - < \nabla_y\phi(x), y >$ vanishes of second order when $y = 0$.

In the analysis of stationary points of the phase we are not interested in time dependence and hence we discard it for this section. Also without loss of generality we assume that the amplitude is compactly supported, more precisely $a \in \mathcal{C}_0^\infty(\mathbb{R}^{n+m})$. Nevertheless, to be able to impose Theorem 1 we need to handle the non-compactness of $\operatorname{supp}(f(x,\xi,y))$ with respect to $\xi \in \mathbb{R}^n$ where $f(x,\xi,y) = \sqrt{|\xi|^2+1}\, a(x+y)$. In order to over come this problem we introduce the infinitely many differentiable cut-off function $\chi(\xi)$ which satisfies

$$\begin{aligned} &\chi(\xi) = 1, && \text{in } W \ni \xi = \nabla_y \phi, \\ &\chi(\xi) = 0, && \text{in } \mathbb{R}^n \setminus \tilde{W}, \quad W \subset\subset \tilde{W} \subset\subset \mathbb{R}^n. \end{aligned}$$

Thus, we rewrite the integral (2.2.1) by splitting into two parts as follows:

$$\begin{aligned} &\int\int \sqrt{|\xi|^2+1}\ a(y+x) e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon} \mathrm{d}\xi \mathrm{d}y \\ &= \int\int (1-\chi(\xi))\sqrt{|\xi|^2+1}\ a(y+x) e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon} \mathrm{d}\xi \mathrm{d}y \\ &\quad + \int\int \chi(\xi)\sqrt{|\xi|^2+1}\ a(y+x) e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon} \mathrm{d}\xi \mathrm{d}y \\ &=: A + B. \end{aligned}$$

We deal with A and B separately. First, using the integration by parts, we are able to show that part A is "sufficiently small" (at least $O(\varepsilon^{2n})$), and then proceed with the stationary phase method for the part B by employing Theorem 1.
To avoid unnecessary complications, first we do it in $n = 1$ and $n = 2$. We hope the idea will be clear for higher dimensions.

(i) *case* $n = 1$:
Observing the identity (keeping in mind that $\xi \neq \partial_y \phi$ on $\mathbb{R} \setminus W$)

$$e^{iS/\varepsilon} = \frac{\varepsilon}{iS_y} \partial_y e^{iS/\varepsilon},$$

where $S = \phi(y+x) - y \cdot \xi$ and $S_y = \partial_y \phi - \xi$, we have

$$A = \int_{\mathbb{R}^n \setminus W} \int g(\xi)\ a(y+x) \frac{\varepsilon}{iS_y} \partial_y e^{iS/\varepsilon} \mathrm{d}y \mathrm{d}\xi,$$

where we denote $g(\xi) := (1-\chi(\xi))\sqrt{|\xi|^2+1}$. Now we observe that every integration by parts will gain us a power of ξ in the denominator (which will guarantee the convergence of the integral over ξ) as well as a power of ε. Applying this three times we obtain the following structure:

$$A = -i\varepsilon^3 \int_{\mathbb{R} \setminus W} \int g(\xi) \left(\frac{f_1(x,y)}{(\phi_y - \xi)^3} + \frac{f_2(x,y)}{(\phi_y - \xi)^4} + \frac{f_3(x,y)}{(\phi_y - \xi)^5} \right) \mathrm{d}y \mathrm{d}\xi,$$

where f_k for $k = 1, 2, 3$ are functions of $a(x+y)$ and $\phi(x+y)$ and their derivatives with respect to y. We can easily deduce that

$$|A| \le 2\varepsilon^3 \int \int_{\mathbb{R}\setminus W} \left(f_1(x,y) \frac{\sqrt{\xi^2+1}}{|\phi_y - \xi|^3} + f_2(x,y) \frac{\sqrt{\xi^2+1}}{|\phi_y - \xi|^4} + f_3(x,y) \frac{\sqrt{\xi^2+1}}{|\phi_y - \xi|^5} \right) \mathrm{d}\xi \mathrm{d}y.$$

Observe that the integral above is finite on both $\mathrm{supp}(a(x+y))$ and $\mathbb{R} \setminus W$, and note that the power of ε in $|A|$ is more than sufficient to compensate the "big" constant in front of the integral (2.2.1) (in case of $n = 1$).

(ii) case $n = 2$:
Similarly, in this case we use

$$e^{iS/\varepsilon} = \frac{\varepsilon}{iS_{y_j}} \partial_{y_j} e^{iS/\varepsilon}, \qquad j = 1, 2,$$

where again $S = \phi(y+x) - y \cdot \xi$ and $S_{y_j} = \partial_{y_j}\phi - \xi_j$, for $j = 1, 2$, and then

$$A = \int_{\mathbb{R}^2\setminus W} \int g(\xi_1, \xi_2)\ a(y_1 + x_1, y_2 + x_2) \frac{\varepsilon}{iS_{y_1}} \cdot \partial_{y_1} e^{iS/\varepsilon} \mathrm{d}y_1 \mathrm{d}y_2 \mathrm{d}\xi_1 \mathrm{d}\xi_2.$$

After three times integration by parts with respect to y_1 we obtain:

$$\begin{aligned} A = -\, i\varepsilon^3 \int_{\mathbb{R}^2\setminus W} \int g(\xi_1, \xi_2) & \left(\frac{f_1(x,y)}{(\phi_{y_1} - \xi_1)^3} + \frac{f_2(x,y)}{(\phi_{y_1} - \xi_1)^4} \right. \\ & \left. + \frac{f_3(x,y)}{(\phi_{y_1} - \xi_1)^5} \right) e^{iS/\varepsilon} \mathrm{d}y_1 \mathrm{d}y_2 \mathrm{d}\xi_1 \mathrm{d}\xi_2, \end{aligned}$$

where as before f_k for $k = 1, 2, 3$ are functions of the amplitude a and the phase ϕ and their derivatives with respect to y_1. Since the integrand is well-behaved with respect to the variable ξ_1, now we are to handle the convergence with respect to ξ_2 (of the integral) by using the integration by parts over y_2. In order to keep the notation as plain as possible we use the shorthand notation $h(x, y, \xi_1)$ instead of the inside of the parenthesis in the integral above. Then again after three times integration by parts with respect to y_2 we obtain,

$$\begin{aligned} A = -\, \varepsilon^6 \int_{\mathbb{R}^2\setminus W} \int g(\xi_1, \xi_2) & \left(\frac{h_1(x,y,\xi_1)}{(\phi_{y_2} - \xi_2)^3} + \frac{h_2(x,y,\xi_1)}{(\phi_{y_2} - \xi_2)^4} \right. \\ & \left. + \frac{h_3(x,y,\xi_1)}{(\phi_{y_2} - \xi_2)^5} \right) e^{iS/\varepsilon} \mathrm{d}y_1 \mathrm{d}y_2 \mathrm{d}\xi_1 \mathrm{d}\xi_2, \end{aligned}$$

where now h_k for $k = 1, 2, 3$ are functions of the amplitude a, phase ϕ, their derivatives with respect to y_1 and y_2 and of $1/(\phi_{y_1} - \xi_1)$. As we deduce in the

$n = 1$ case we obtain that $|A| \sim O(\varepsilon^6)$. From here it is not hard to conclude that in the n-dimension case we will obtain

$$|A| \sim O(\varepsilon^{3n}),$$

which concludes that the contribution to the oscillating integral (2.2.1) from the part A is "small", more precisely of order $O(\varepsilon^{2n})$.

For the part B we employ Theorem 1 which provides an expansion for the integral (2.2.1) of order $O(\varepsilon)$. We obtain

$$\begin{aligned}&\int\int \chi(\xi)\sqrt{|\xi|^2+1}\; a(y+x)e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon}\mathrm{d}y\mathrm{d}\xi \\ &\approx e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n \sum_{\nu=0}^{3} \frac{1}{\nu!} < i\varepsilon D_y, D_\xi >^\nu \left(e^{ir_x(y)/\varepsilon}\sqrt{|\xi|^2+1}\; a(y+x)\right)\Bigg|_{\substack{y=0,\\ \xi=\nabla_y\phi(x)}}\end{aligned} \tag{2.2.2}$$

where $r_x(y) = \phi(y+x) - \phi(x) - \nabla_y\phi(x)\cdot y$, and it is clear that if we expand until $\nu = k - n = 3$, then the difference between the two sides of (2.2.2) is bounded by

$$C\varepsilon^{n+3/2} \sum_{|\alpha|\leq 2k} \sup_{y,\xi} \mid D^\alpha_{y,\xi} u(y,\xi,x) \mid .$$

This will ensure that the oscillatory integral (2.2.1) will be approximated with an error of order $O(\varepsilon)$. For the convenience of the reader we give the computations explicitly (see appendix 2.A). Eventually, what we get from the expansion (2.2.2) is as follows

$$\begin{aligned}&\int\int \sqrt{|\xi|^2+1}\; a(y+x)e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon}dyd\xi \\ &\approx e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n \Bigg[a\sqrt{|\nabla_y\phi|^2+1} \\ &-i\varepsilon\left(\frac{\nabla_y\phi\cdot\nabla_y a}{\sqrt{|\nabla_y\phi|^2+1}} + \frac{a\Delta\phi}{\sqrt{|\nabla_y\phi|^2+1}} - \sum_{j=1}^{n}\frac{\phi_{y_j}(\nabla_y\phi\cdot(\nabla_y\phi)_{y_j})}{(|\nabla_y\phi|^2+1)}\right)\Bigg] \\ &= e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n\left[a\sqrt{|\nabla_y\phi|^2+1} - i\varepsilon\mathrm{div}\left(\frac{a^2\nabla_y\phi}{\sqrt{|\nabla_y\phi|^2+1}}\right)\frac{1}{2a}\right]\end{aligned}$$

with an error of order $O(\varepsilon)$ as we aimed to obtain.

2.3 The WKB-system

In order to obtain the corresponding system, we plug the ansatz (2.1.6) into the evolution equation (2.1.1) and use the expansion given by Theorem 1 in Section 2.2 for the oscillatory integral, and then we obtain

$$\varepsilon\partial_t a + ia\partial_t\phi + ia\sqrt{|\nabla_y\phi|^2+1} + \varepsilon\mathrm{div}\left(\frac{a^2\nabla_y\phi}{\sqrt{|\nabla_y\phi|^2+1}}\right)\frac{1}{2a} = O(\varepsilon).$$

In leading order terms if we split the real and imaginary parts, then this yields a system of equations written in terms of the density $n(x,t) = (a(x,t))^2$ and the phase function $\phi(x,t)$ in an asymptotic description:

$$\begin{aligned}\partial_t n + \mathrm{div}\left(\frac{n\nabla_y\phi}{\sqrt{|\nabla_y\phi|^2+1}}\right) &= 0,\\ \partial_t\phi + \sqrt{|\nabla_y\phi|^2+1} &= 0.\end{aligned}$$

Here the first equation is a conservation law written for the density $n(x,t)$ (or a transport equation for the amplitude $a(x,t)$) and the latter one is a Hamilton-Jacobi equation for the phase $\phi(x,t)$. As a last remark we point out that the solutions to this system are only local-in-time because of the characteristics of the Hamilton-Jacobi equation.

2.A Computations in the expansion (2.2.2)

First we note that since the cut-off function $\chi(\xi)$ satisfies the following:

(i) $\chi(\xi) = 1$

(ii) $\chi'(\xi) = 0$

on $W \ni y = \nabla_y\phi$ it has no effect to the following computations. Thus we discard χ in the calculations. Now, let us compute the terms in the expansion corresponding each case of $\nu = 0, 1, 2, 3$:

$$\begin{aligned}\nu = 0: \quad & e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n\left(e^{ir_x(y)/\varepsilon}\sqrt{|\xi|^2+1}\;a(y+x)\right)\Big|_{\substack{y=0,\\ \xi=\nabla_y\phi(x)}}\\ & = (2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon}a(x)\sqrt{|\nabla_y\phi(x)|^2+1}.\end{aligned}$$

And since $D_y, D_\xi \in \mathbb{R}^n$ then $< i\varepsilon D_y, D_\xi >= -i\varepsilon \sum_{j=1}^n \partial_{y_j}\partial_{\xi_j}$. So,

$$\nu = 1 :$$
$$- i(2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon}\varepsilon \sum_{j=1}^n \partial_{y_j}\partial_{\xi_j}\left(e^{ir_x(y)/\varepsilon}\sqrt{|\xi|^2+1}\; a(y+x)\right)\Big|_{\substack{y=0,\\ \xi=\nabla_y\phi(x)}} . \tag{2.A.1}$$

Let us calculate the derivatives:

$$\star\ \ \partial_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1} = e^{ir_x(y)/\varepsilon} a(y+x)\frac{\xi_j}{\sqrt{|\xi|^2+1}},$$

$$\begin{aligned}\star\ \ &\partial_{y_j}\partial_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}\\ &= \frac{\xi_j}{\sqrt{|\xi|^2+1}}\partial_{y_j}\left(e^{ir_x(y)/\varepsilon} a(y+x)\right)\\ &= \frac{\xi_j}{\sqrt{|\xi|^2+1}}\left(\frac{i}{\varepsilon}a(y+x)\partial_{y_j} r_x(y) + a_{y_j}(y+x)\right)e^{ir_x(y)/\varepsilon}\end{aligned}$$

where $\partial_{y_j} r_x(y) = \phi_{y_j}(y+x) - \phi_{y_j}(x)$ and equals to zero at $y=0$. If we rewrite (2.A.1) then,

$$\begin{aligned}&\nu = 1 :\\ &- i(2\pi\varepsilon)^n \varepsilon e^{i(\phi(x)+r_x(y))/\varepsilon}\sum_{j=1}^n \frac{\xi_j}{\sqrt{|\xi|^2+1}}\left(\frac{i}{\varepsilon}\partial_{y_i} r_x(y) a(y+x) + a_{y_j}(y+x)\right)\Big|_{\substack{y=0,\\ \xi=\nabla_y\phi(x)}}\\ &= -i(2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon}\varepsilon\sum_{j=1}^n \frac{\phi_{y_j}(x)}{\sqrt{\left|\nabla_y\phi(x)\right|^2+1}} a_{y_j}(x)\\ &= -i(2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon}\varepsilon\frac{\nabla_y\phi(x)\cdot\nabla_y a(x)}{\sqrt{|\nabla_y\phi(x)|^2+1}}.\end{aligned}$$

Next we compute the contributions from the third term. The explicit form of $< i\varepsilon D_y, D_\xi >^2$ is given by

$$\begin{aligned}< i\varepsilon D_y, D_\xi >^2 &= -\varepsilon^2\Bigg(\sum_{j=1}^n(\partial_{y_j}\partial_{\xi_j})^2 + \sum_{j=1}^n\sum_{\substack{k=1\\ j\neq k}}^n \partial_{y_j}\partial_{\xi_j}\partial_{y_k}\partial_{\xi_k}\Bigg)\\ &=: -\varepsilon^2\Bigg(\sum D_1 + \sum\sum D_2\Bigg). \qquad (2.A.2)\end{aligned}$$

Then D_1 acts as

$$D_1 e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}$$

$$= \partial^2_{y_j}\partial^2_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}$$

$$= \frac{(|\xi|^2+1)-\xi_j\xi_j}{(|\xi|^2+1)^{3/2}} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\left(\frac{i}{\varepsilon}\partial_{y_i} r_x(y) a(y+x) + a_{y_j}(y+x)\right)\partial_{y_j} r_x(y)\right.$$

$$\left. + \frac{i}{\varepsilon}\left(\phi_{y_j y_j}(y+x) a(y+x) + \partial_{y_i} r_x(y) a_{y_j}(y+x)\right) a_{y_j y_j}(y+x)\right],$$

since

$$\partial_{y_j}\partial^2_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}$$

$$= \partial_{\xi_j}\frac{\xi_j}{\sqrt{|\xi|^2+1}} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\left(\phi_{y_j}(y+x) - \phi_{y_j}(x)\right) a(y+x) + a_{y_j}(y+x)\right]$$

$$= \frac{(|\xi|^2+1)-\xi_j\xi_j}{(|\xi|^2+1)^{3/2}} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\partial_{y_i} r_x(y) a(y+x) + a_{y_j}(y+x)\right]$$

and

$$\partial^2_{y_j}\partial^2_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}$$

$$= \frac{(|\xi|^2+1)-\xi_j\xi_j}{(|\xi|^2+1)^{3/2}}\partial_{y_j}\left(e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\left(\phi_{y_j}(y+x) - \phi_{y_j}(x)\right) a(y+x) + a_{y_j}(y+x)\right]\right).$$

And for the part D_2 in (2.A.2) we have to evaluate

$$\partial_{\xi_k}\partial_{y_j}\partial_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}$$

$$= \partial_{\xi_k}\frac{\xi_j}{\sqrt{|\xi|^2+1}} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\partial_{y_i} r_x(y) a(y+x) + a_{y_j}(y+x)\right]$$

$$= \frac{-\xi_j\xi_k}{\left(|\xi|^2+1\right)^{3/2}} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\partial_{y_i} r_x(y) a(y+x) + a_{y_j}(y+x)\right]$$

and

$$D_2 e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1} = \partial_{y_k}\partial_{\xi_k}\partial_{y_j}\partial_{\xi_j} e^{ir_x(y)/\varepsilon} a(y+x)\sqrt{|\xi|^2+1}$$

$$= \frac{-\xi_j\xi_k}{\left(|\xi|^2+1\right)^{3/2}}\partial_{y_k} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon} a(y+x)\partial_{y_j} r_y(x) + a_{y_j}(y+x)\right]$$

$$= \frac{-\xi_j\xi_k}{\left(|\xi|^2+1\right)^{3/2}} e^{ir_x(y)/\varepsilon}\left[\frac{i}{\varepsilon}\left(\frac{i}{\varepsilon} a(y+x)\partial_{y_j} r_x(y) + a_{y_j}(y+x)\right)\partial_{y_k} r_y(x)\right.$$

$$\left. + \frac{i}{\varepsilon} a(y+x)\partial^2_{y_k y_j} r_y(x) + \frac{i}{\varepsilon} a_{y_k}(y+x)\partial_{y_j} r_y(x) + a_{y_j y_k}(y+x)\right]$$

where $\partial^2_{y_k y_j} r_y(x) = \phi_{y_j y_k}$. Consequently, the third term gives

$$\nu = 2:$$

$$(2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon} \sum_{j=1}^n \frac{1}{2} < i\varepsilon D_y, D_\xi >^2 \left(e^{i r_x(y)/\varepsilon} \sqrt{|\xi|^2+1}\; a(y+x) \right) \Big|_{\substack{y=0,\\ \xi=\nabla_y\phi(x)}}$$

$$= -\frac{\varepsilon^2}{2}(2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon} \left[\sum_{j=1}^n \frac{(|\nabla_y\phi|^2+1) - \phi_{y_j}\phi_{y_j}}{(|\nabla_y\phi|^2+1)^{3/2}} \left[\frac{i}{\varepsilon}\phi_{y_j y_j}(x) a(x) + a_{y_j y_j}(x) \right] \right.$$

$$\left. - \sum_{j=1}^n \sum_{\substack{k=1\\ j\neq k}}^n \frac{\phi_{y_j}\phi_{y_k}}{(|\nabla_y\phi|^2+1)^{3/2}} \left(\frac{i}{\varepsilon} a(x)\phi_{y_k y_j}(x) + a_{y_j y_k}(x) \right) \right]$$

since $r_x(0) = 0$ and $\partial_{y_j} r_x(y) \mid_{y=0} = 0$. If we arrange it considering the order, we obtain

$$\nu = 2: \qquad = -(2\pi\varepsilon)^n e^{i\phi(x)/\varepsilon} \left[\frac{i\varepsilon}{2} \left(\frac{a(x)}{(|\nabla_y\phi|^2+1)^{1/2}} \sum_{j=1}^n \phi_{y_j y_j} \right.\right.$$

$$\left. - \frac{a(x)}{(|\nabla_y\phi|^2+1)^{3/2}} \sum_{j=1}^n \left(\phi_{y_j y_j}\phi_{y_j}\phi_{y_j} + \phi_{y_j} \sum_{\substack{k=1\\ j\neq k}}^n \phi_{y_k y_j}\phi_{y_k} \right) \right)$$

$$\left. + O(\varepsilon^2) \right]. \quad (2.A.3)$$

It is clear that

$$\phi_{y_j y_j}\phi_{y_j}\phi_{y_j} + \phi_{y_j} \sum_{\substack{k=1\\ j\neq k}}^n \phi_{y_k y_j}\phi_{y_k} = \phi_{y_j} \sum_{k=1}^n \phi_{y_k y_j}\phi_{y_k} = \phi_{y_j} \left(\nabla_y\phi \cdot (\nabla_y\phi)_{y_j} \right)$$

and consequently,

$$\nu = 2:$$

$$= (2\pi\varepsilon)^n \left[-i\varepsilon \frac{a(x)e^{i\phi(x)/\varepsilon}}{(|\nabla_y\phi|^2+1)^{1/2}} \left(\sum_{j=1}^n \phi_{y_j y_j} - \frac{\phi_{y_j}\left(\nabla_y\phi \cdot (\nabla_y\phi)_{y_j} \right)}{(|\nabla_y\phi|^2+1)} \right) + O(\varepsilon^2) \right].$$

It only remains to compute the derivatives from the term $\langle i\varepsilon D_y, D_x i\rangle^3$ but since there will be no contribution from this term of order $O(\varepsilon)$ (which can be realized post facto) we omit this computation. Eventually, we can deduce from what we obtained above that

$$
\begin{aligned}
&\int\int \sqrt{|\xi|^2+1}\; a(y+x)e^{i(\phi(y+x)-y\cdot\xi)/\varepsilon}dyd\xi \\
&\quad\approx e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n\left[a\sqrt{\left|\nabla_y\phi\right|^2+1}\right. \\
&\quad\left.-i\varepsilon\left(\frac{\nabla_y\phi\cdot\nabla_y a}{\sqrt{\left|\nabla_y\phi\right|^2+1}}+\frac{a\Delta\phi}{\sqrt{\left|\nabla_y\phi\right|^2+1}}-\sum_{j=1}^{n}\frac{\phi_{y_j}(\nabla_y\phi\cdot(\nabla_y\phi)_{y_j})}{(\left|\nabla_y\phi\right|^2+1)}\right)\right] \\
&\quad= e^{i\phi(x)/\varepsilon}(2\pi\varepsilon)^n\left[a\sqrt{\left|\nabla_y\phi\right|^2+1}-i\varepsilon\mathrm{div}\left(\frac{a^2\nabla_y\phi}{\sqrt{\left|\nabla_y\phi\right|^2+1}}\right)\frac{1}{2a}\right]
\end{aligned}
$$

with an error of order $O(\varepsilon)$ as we aimed to obtain.

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Chapter 3

Classical limit for semi-relativistic Hartree systems *

3.1 Introduction

3.1.1 Mathematical setting of the model

We consider the *semi-relativistic Hartree system* (or Schrödinger-Poisson system) in the semi-classical regime, i.e.

$$\begin{cases} i\varepsilon \dfrac{\mathrm{d}}{\mathrm{d}t}\rho^\varepsilon(t) = [H^\varepsilon, \rho^\varepsilon(t)], \quad x \in \mathbb{R}^3,\, t \in \mathbb{R}_+, \\ -\kappa \Delta V^\varepsilon = n^\varepsilon(t,x), \quad \kappa = \pm 1, \end{cases} \tag{3.1.1}$$

subject to an initial data $\rho^\varepsilon(0) \equiv \rho_0^\varepsilon$, where the reason for choosing $\kappa = \pm 1$ respectively will be explained below and the Hamiltonian operator H^ε is given by

$$H^\varepsilon := \sqrt{-\varepsilon^2\Delta + 1} + V^\varepsilon(t,x).$$

Here the pseudo-differential operator for the kinetic energy is simply defined via multiplication in Fourier space with the symbol $\sqrt{|\varepsilon\xi|^2 + 1}$ which has been given explicitly in the previous chapter, for the semi-classical parameter $0 < \varepsilon \ll 1$, a dimensionless scaled Planck's constant (all other physical constants are rescaled to be equal to 1). This scalar pseudo-differential operator is frequently used in relativistic quantum mechanical models as a convenient replacement of the full (matrix-valued) Dirac operator. In (3.1.1) we denote by $\rho^\varepsilon(t) \in \mathfrak{S}_1(L^2(\mathbb{R}^3))$ the density matrix operator of the system, i.e. a positive self-adjoint trace class operator acting on $L^2(\mathbb{R}^3)$. The particle density $n^\varepsilon(t,\cdot) \in L^1(\mathbb{R}^3)$ is then obtained

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by evaluating the corresponding kernel $\rho^\varepsilon(t,x,y)$, which, by abuse of notation is denoted by the same symbol as the density operator, on its diagonal [30], i.e. $n^\varepsilon(t,x) = \rho^\varepsilon(t,x,x)$. The system (3.1.1) describes the *mean field dynamics* of (semi-relativistic) quantum mechanical particles in a *mixed state* which are the statistical mixture of pure states. In the system (3.1.1) operators (observables) evolve in time where states of the system are constants. That means for a system in a fixed state one can make measurements on the observables (like momentum or position). This representation is called *Heisenberg picture*. Since $\rho(t)$ is a self-adjoint and compact operator it has a discrete spectrum, i.e. denoting by $\{\psi_j^\varepsilon\}_{j\in\mathbb{N}}$ a complete orthonormal basis of $L^2(\mathbb{R}^3)$ we can decompose the kernel of $\rho^\varepsilon(t) \in \mathfrak{S}_1(L^2(\mathbb{R}^3))$ via

$$\rho^\varepsilon(t,x,y) = \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon\, \psi_j^\varepsilon(t,x)\overline{\psi_j^\varepsilon}(t,y),$$

with (constant in time) $\lambda_j \in \ell^1$, $\lambda_j \geq 0$ [30]. Using this representation, we arrive at an *equivalent* system of countable many nonlinear Schrödinger-type equations

$$\begin{cases} i\varepsilon\partial_t\psi_j^\varepsilon = \sqrt{-\varepsilon^2\Delta + 1}\;\psi_j^\varepsilon + V^\varepsilon(t,x)\psi_j^\varepsilon \\ -\kappa\Delta V^\varepsilon = n^\varepsilon(t,x), \end{cases} \tag{3.1.2}$$

where the density is now given by

$$n^\varepsilon(t,x) = \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon |\psi_j^\varepsilon(t,x)|^2.$$

This approach which is a system written for the time-dependent states that produce the same result of a fixed observable (i.e. an observable has a fixed value in the system) is called *Schrödinger picture*. The system (3.1.2) can be interpreted as the time-dependent model associated to the semi-relativistic *Hartree energy*

$$\begin{aligned} \mathcal{E}_{\mathrm{H}}^\varepsilon(t) &= \mathcal{E}_{\mathrm{kin}}^\varepsilon(t) + \mathcal{E}_{\mathrm{pot}}^\varepsilon(t) \\ &= \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon \|(-\varepsilon^2\Delta + 1)^{1/4}\psi_j^\varepsilon\|_{L^2(\mathbb{R}^3)}^2 + \frac{\kappa}{8\pi}\iint_{\mathbb{R}^6} \frac{n^\varepsilon(t,x)n^\varepsilon(t,y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y, \end{aligned}$$

where for the second line we have used the three dimensional Green's function representation of the potential, i.e.

$$V^\varepsilon(t,x) = \frac{\kappa}{4\pi|x|} * n^\varepsilon(t,x).$$

For future references we recall that the kinetic and the self-consistent potential-energy can also be shortly written in terms of density matrices as

$$\mathcal{E}_{\mathrm{kin}}^\varepsilon(t) = \mathrm{tr}(\sqrt{-\varepsilon^2\Delta + 1}\;\rho^\varepsilon(t)), \quad \mathcal{E}_{\mathrm{pot}}^\varepsilon(t) = \frac{\kappa}{2}\,\mathrm{tr}(V^\varepsilon(t,x)\rho^\varepsilon(t)).$$

In the case $\kappa = -1$, the coupling to the Poisson equation comprises an *attractive nonlinearity* for the Schrödinger-type equations (3.1.2) and hence, global well-posedness for general initial data does not hold, cf. [6, 11]. In this case, the system (3.1.2) is a generalization (for mixed states) of the semi-relativistic Hartree model derived in [3] as the mean field limit for large systems of Bosons with gravitational self-interaction. This model has been extensively studied in recent years as it is considered to describe the dynamics of so-called *Boson stars* [5, 6, 7, 11]. In the case $\kappa = 1$, the Poisson interaction is *repulsive* and typically models electron-electron self-interactions (in the Hartree-approximation). The system (3.1.2) therefore allows to study relativistic corrections to the usual Hartree model of many-body electron system as it is needed for example in the case of heavy atoms, cf. [14].

Throughout this chapter, we shall use the following definition for the Fourier transform

$$(\mathcal{F}_{\xi \to \eta} \varphi)(\eta) = \int_{\mathbb{R}^3} \varphi(\xi) e^{-i\xi \cdot \eta} \, \mathrm{d}\xi.$$

Moreover we denote by $\mathcal{S}$ the Schwartz space of rapidly decaying functions.

In the following subsection we give a brief introduction to the Wigner transform and Wigner measures, see [28], which will turn out to be very useful tool for the semi-classical limit we want to carry.

3.1.2 Wigner measures

As we have stated before, in this chapter of the thesis, we are interested in rigorously establishing the classical limit of (3.1.2) as $\varepsilon \to 0$ which is nontrivial since the limits are weak limits due to the oscillations (as we have seen in the previous chapter) and concentrations. In particular, we want to investigate the convergence behavior in the limit $\varepsilon \to 0$ of quadratic quantities, i.e. position densities etc. To understand it let us take a sequence of wavefunctions $(\psi^\varepsilon(x))$ that is uniformly bounded in $L^2(\mathbb{R}^3)$. By compactness theorem, we can extract a weak-$*$ (i.e. weakly, in $L^2(\mathbb{R}^3)$) convergent subsequence with the limit $\psi^0(x)$. For a moment let us assume that we consider the system (3.1.1) in a pure state where the quadratic quantity (density) is given by $n^\varepsilon(x) = |\psi^\varepsilon(x)|^2$. Clearly, $n^\varepsilon(x)$ is also uniformly bounded in $L^p(\mathbb{R}^3)$ for some $p > 1$ and converges weak-$*$ to some $n^0(x) = \lim_{\varepsilon \to 0} |\psi^\varepsilon(x)|^2$. Intrinsically, "the square of the weak limit is not the weak limit of the square": $n^0(x) \neq |\psi^0(x)|$. A similar obstacle also arises for the nonlinear term involving $V^\varepsilon(t,x)$ in establishing a limiting point in an appropriate sense.

As a convenient mathematical tool to deal with the weak convergence of the quadratic quantities, we shall heavily rely on the Wigner transformed picture of quantum mechanics [28]. The Wigner measure can be seen as a tool that measures the lack of compactness that inhibits the sequence $\psi^\varepsilon(x)$ from converging strongly in $L^2(\mathbb{R}^3)$. Thus, as in [11], we define the (ε-scaled) *Wigner transform*, for $g, h \in \mathcal{S}'(\mathbb{R}^3)$,

$$f^\varepsilon(g,h)(x,\xi) := \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} g\left(x+\frac{\varepsilon y}{2}\right)\bar{h}\left(x-\frac{\varepsilon y}{2}\right)e^{-i\xi\cdot y}\,\mathrm{d}y.$$

For fixed ε, this clearly defines a continuous bilinear mapping from $\mathcal{S}'(\mathbb{R}^3)\times\mathcal{S}'(\mathbb{R}^3)$ to $\mathcal{S}'(\mathbb{R}^3\times\mathbb{R}^3)$. In the sequel of this section we will give a brief introduction to the Wigner transformation by following [11], Section 1. We start with one of the crucial properties:

Proposition 3.1.1 (see [11])**.** *If g and h lie in a bounded subset of $L^2(\mathbb{R}^3_x)$, then $f^\varepsilon(g,h)$ lie in a bounded subset of $\mathcal{S}'(\mathbb{R}^3_x\times\mathbb{R}^3_\xi)$. More precisely, we have for the respective Fourier transforms*

$$\begin{aligned}(\mathcal{F}_{\xi\to v}f^\varepsilon(g,h))(x,v) &\in C_0(\mathbb{R}^3_v;L^1(\mathbb{R}^3_x)),\\ (\mathcal{F}_{x\to\zeta}f^\varepsilon(g,h))(\zeta,\xi) &\in C_0(\mathbb{R}^3_\zeta;L^1(\mathbb{R}^3_\xi))\end{aligned}$$

with the respective norms bounded by $\|g\|_{L^2}\|h\|_{L^2}$.

Further, we have the following estimate for $a, b \in \mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$

$$\left\langle f^\varepsilon(g,h), a\bar{b}\right\rangle = \int_{\mathbb{R}^3}(a(x,\varepsilon D_x)g)\overline{(b(x,\varepsilon D_x)h)}\mathrm{d}x + r_\varepsilon, \tag{3.1.3}$$

where $|r_\varepsilon| \le \varepsilon C(a,b)\|g\|_{L^2}\|h\|_{L^2}$.

The estimate (3.1.3) *holds analogously for the Weyl operators $a^W(x,\varepsilon D_x)$, $b^W(x,\varepsilon D_x)$ instead of $a(x,\varepsilon D_x)$, $b(x,\varepsilon D_x)$ on the right-hand side. By C_0 we denote zero-at-infinity continuous functions.*

Remark 3.1.2. Basic properties of the Wigner transform are

$$\begin{aligned}\int_{\mathbb{R}^3} f^\varepsilon(g,h)\mathrm{d}\xi &= g(x)\bar{h}(x)\\ \int_{\mathbb{R}^3} f^\varepsilon(g,h)\mathrm{d}x &= \frac{1}{(2\pi\varepsilon)^\varepsilon}\hat{g}\left(\frac{\xi}{\varepsilon}\right)\bar{\hat{h}}\left(\frac{\xi}{\varepsilon}\right).\end{aligned}$$

The duality in x and ξ can be expressed, for example, as

$$f^\varepsilon(g,h)(x,\xi) = f^\varepsilon\left(\frac{1}{(2\pi\varepsilon)^{\varepsilon/2}}\bar{\hat{h}}\left(\frac{\cdot}{\varepsilon}\right), \frac{1}{(2\pi\varepsilon)^{\varepsilon/2}}\bar{\hat{g}}\left(\frac{\cdot}{\varepsilon}\right)\right)(\xi,x). \tag{3.1.4}$$

In general, one can define for g, h in $\mathcal{S}'(\mathbb{R}^3)^n$ an $n \times n$ "Wigner matrix" by

$$F^\varepsilon(g,h)(x,\xi) := \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} g\left(x + \frac{\varepsilon y}{2}\right) \otimes \bar{h}\left(x - \frac{\varepsilon y}{2}\right) e^{-i\xi\cdot y}\, \mathrm{d}y$$

where $\otimes$ denotes the tensor product of vectors.

As a special case, let (g^ε) be a bounded family in $L^2(\mathbb{R}^3)^n$. Then we denote by $F^\varepsilon[g^\varepsilon]$ the $n \times n$ matrix whose elements are given by

$$f_{ij}^\varepsilon[g^\varepsilon] = f^\varepsilon(g_i^\varepsilon, g_j^\varepsilon).$$

Also, we denote by $f^\varepsilon[g^\varepsilon] = \operatorname{tr} F^\varepsilon[g^\varepsilon]$ the scalar Wigner transform of g^ε.

By (3.1.4), $F^\varepsilon[g^\varepsilon]$ is self-adjoint, and by Proposition 2.1. there exists a subsequence that is convergent in $\mathcal{S}'$. Let F^0 be that limit. It can be proven that F^0 is a nonnegative matrix-valued measure; that is, for any $z \in \mathcal{C}^n$, we have

$$\bar{z}F^0 z \geq 0 \qquad \Leftrightarrow \qquad \sum_{i,j} f_{ij}^0 z_i \bar{z}_j \geq 0 \tag{3.1.5}$$

as a measure. Since for every nonnegative function $a \in C_0^\infty$ there exists some sequence (b_n) in C_0^∞ such that, a is the limit of $|b_n|^2$, it is sufficient to prove

$$\sum_{i,j} \langle f_{ij}^0, |b|^2 \rangle z_i \bar{z}_j \geq 0 \qquad b \in C_0^\infty.$$

This fact can be observed by using (3.1.3) in Proposition 2.1.:

$$\sum_{i,j} \langle f^\varepsilon(g_i^\varepsilon, g_j^\varepsilon), z_i \bar{z}_j |b|^2 \rangle = \int_{\mathbb{R}^3} \left| \sum_i z_i b(x, \varepsilon D) g_i^\varepsilon \right|^2 \mathrm{d}x + O(\varepsilon).$$

By passing to the limit, (3.1.5) is proved.

Remark 3.1.3. Some other proofs for the positivity of the limiting Wigner measures can be found in [10, 19, 20, 21] where a Gaussian regularization (Husimi function)

$$f_H^\varepsilon[g^\varepsilon] := f^\varepsilon[g^\varepsilon] * G^\varepsilon *_\xi G^\varepsilon, \qquad G^\varepsilon(z) := \frac{1}{(\pi\varepsilon)^{3/2}} e^{-|z|^2/2}$$

is used, which is a pointwise nonnegative function. Since the accumulation points of $f^\varepsilon[g^\varepsilon]$ are also accumulation points of $f_H^\varepsilon[g^\varepsilon]$, one concludes that f^0 is a nonnegative measure.

In order to investigate the relationship between the Wigner measure and the weak limits of quadratic forms of g^ε, we need two definitions.

Definition 3.1.4. A bounded family (g^ε) in L^2 is said to be ε-*oscillatory* as ε goes to 0 if the following property holds for every continuous, compactly supported function φ on $\mathbb{R}^3$:

$$\overline{\lim_{\varepsilon\to 0}} \int_{|\xi|\geq R/\varepsilon} |\widehat{\varphi g^\varepsilon}(\xi)|^2 \mathrm{d}\xi \longrightarrow 0 \qquad \text{as} \;\; R \;\; \text{goes to} \;\; +\infty.$$

This heuristically means that the wavelength of oscillations of g^ε is at least of order ε. Note that the condition

$$\exists \kappa > 0 \quad \text{such that} \quad \varepsilon^\kappa D^\kappa g^\varepsilon \text{uniformly bounded in} \quad L^2_{\text{loc}} \tag{3.1.6}$$

is sufficient for a function to be ε-oscillatory.

A bounded family (g^ε) in L^2 is said to be *compact* at infinity as ε goes to 0 if

$$\overline{\lim_{\varepsilon\to 0}} \int_{|\xi|\geq R/\varepsilon} |g^\varepsilon(x)|^2 \mathrm{d}x \longrightarrow 0 \qquad \text{as} \;\; R \;\; \text{goes to} \;\; +\infty.$$

Now we can state the following result from [11]:

Proposition 3.1.5. *Let (g^ε) be a bounded family in $L^2(\mathbb{R}^3)$ with a Wigner measure f^0. Then we have*

$$f^0(\mathbb{R}^3\times\mathbb{R}^3) = \int_{\mathbb{R}^6} f^0(x,\xi)\mathrm{d}x\mathrm{d}\xi \leq \overline{\lim_{\varepsilon\to 0}} \int_{\mathbb{R}^3} |g^\varepsilon(x)|^2 \mathrm{d}x \tag{3.1.7}$$

with equality if and only if (g^ε) is ε-oscillatory and compact at infinity. In this case $\overline{\lim}$ can be replaced by lim *in the right-hand side of* (3.1.7).

Here we note that same results also have been obtained in several papers, for instance see [19], Theorem III.2., [20], Lemma 3.1.

Eventually, we denote the Wigner function of a given density matrix kernel $\rho^\varepsilon(t,x,y)$ as in [20, 19]

$$f^\varepsilon[\rho^\varepsilon(t)] \equiv f^\varepsilon(t,x,\xi) := \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \rho^\varepsilon\left(t, x+\frac{\varepsilon y}{2}, x-\frac{\varepsilon y}{2}\right) e^{-i\xi\cdot y}\, \mathrm{d}y,$$

From this definition we easily infer

$$\|f^\varepsilon(t,\cdot,\cdot)\|^2_{L^2(\mathbb{R}^3_x\times\mathbb{R}^3_\xi)} = (2\pi\varepsilon)^{-3} \|\rho^\varepsilon(t,\cdot,\cdot)\|^2_{L^2(\mathbb{R}^3_x\times\mathbb{R}^3_y)}. \tag{3.1.8}$$

Since $f^\varepsilon(t,x,\xi)$ is real-valued it can be seen as a quantum mechanical analog of a classical phase space distribution. Hence, the Wigner function f^ε satisfies the following kinetic-like evolution equation:

$$\partial_t f^\varepsilon + \Gamma^\varepsilon f^\varepsilon + \Theta^\varepsilon[V^\varepsilon] f^\varepsilon = 0,$$

in the distributional sense. Here, Γ^ε and $\Theta^\varepsilon[V^\varepsilon]$ are pseudo-differential operators, corresponding to the Wigner transformed kinetic and potential energy terms. Explicitly, $\Gamma^\varepsilon f^\varepsilon$ is given by

$$\Gamma^\varepsilon f^\varepsilon(t,x,\xi) = \frac{i}{(2\pi)^3} \iint_{\mathbb{R}^3\times\mathbb{R}^3} e^{iy\cdot(x-\eta)}\ y\cdot\gamma^\varepsilon(y,\xi) f^\varepsilon(t,\eta,\xi)\,\mathrm{d}y\,\mathrm{d}\eta,$$

where

$$\gamma^\varepsilon(y,\xi) := \frac{2\xi}{\sqrt{|\xi+\varepsilon\frac{y}{2}|^2+1}+\sqrt{|\xi-\varepsilon\frac{y}{2}|^2+1}} \in \mathbb{R}^3.$$

On the other hand, the nonlinear potential $V^\varepsilon(t,x)$ enters via the well known operator, cf. [19, 20]

$$\Theta^\varepsilon[V^\varepsilon] f^\varepsilon(t,x,\xi) = \frac{i}{(2\pi)^3} \iint_{\mathbb{R}^3\times\mathbb{R}^3} e^{i\eta\cdot(z-\xi)}\delta^\varepsilon(t,x,\eta) f^\varepsilon(t,x,z)\,\mathrm{d}\eta\,\mathrm{d}z.$$

whose symbol is given by

$$\delta^\varepsilon(t,x,\eta) := \frac{1}{\varepsilon}\Big(V^\varepsilon(t,x+\varepsilon\frac{\eta}{2}) - V^\varepsilon(t,x-\varepsilon\frac{\eta}{2})\Big) = \eta\cdot\int_{-1/2}^{1/2} \nabla_x V^\varepsilon(t,x+\varepsilon s\eta)\,\mathrm{d}s.$$

The Wigner function in general also takes negative values and therefore does not allow for a probabilistic interpretation. Nevertheless, Wigner functions have proved to be a highly successful tool in the rigorous mathematical derivation of classical limits, see, e.g. [1, 9, 11, 19, 20, 24, 26] for various analytical results and [22] for a numerical study. In particular, under appropriate uniform bounds on ρ^ε (see Theorem 1, in Section 3.3), it is known that f^ε has accumulation points $f \equiv f^0(t,x,\xi)$ as $\varepsilon \to 0$ (in a suitable topology), which are positive Borel measures on the phase space. The limiting measures can then be identified as a distributional solution of the corresponding limiting evolutionary system. In our case we expect it to be a solution of the *relativistic Vlasov-Poisson system*, i.e.

$$\begin{cases} \partial_t f + \dfrac{\xi}{\sqrt{|\xi|^2+1}}\cdot\nabla_x f - \nabla_x V\cdot\nabla_\xi f = 0, \\ -\kappa\Delta V = n(t,x), \end{cases} \tag{3.1.9}$$

where the limiting particle density $n(t,x)$ is obtained as

$$n(t,x) = \int_{\mathbb{R}^3} f(t,x,\xi)\,\mathrm{d}\xi.$$

The system (3.1.9) is in itself an intensively studied model, in particular in the gravitational case $\kappa = -1$, see e.g. [12, 13, 14] and the references given therein.

The present work thus provides a rigorous connection between the quantum mechanical model (3.1.1), or equivalently (3.1.2), and its classical analog (3.1.9). The novelty of the work lies in the fact that we have to establish suitable estimates based on the relativistic kinetic energy (instead of the usual one $-\frac{\varepsilon^2}{2}\Delta$) in order to be able to pass to the limit in the nonlinear potential $V^\varepsilon(t,x)$.

The rest of this chapter is now organized as follows: In Section 3.2 we collect some preliminary results (a priori uniform energy bounds, existence, compactness, etc.) needed for the proof of our main theorem which is stated and proven in Section 3.3. We then discuss some possible generalizations concerning the self-consistent potential term and close the Section 3.4 with a final remark.

3.2 Preliminary results

In this section, as well as we establish new interpolation estimates (or Lieb-Thirring type inequalities) which will allow us to access (uniform) bounds in terms of the semi-relativistic kinetic energy, we will give a complete proof of the well-posedness of the Hartree system (3.1.1) for the sake of the completeness of the arguments used. In this concept we also give an explicit compactness argument to be used in the limit procedure pursued in the next section.

3.2.1 Interpolation estimates

Let us start with a technical lemma, that nevertheless turns out to be crucial for the proof of the main Theorem.

Lemma 3.2.1. *Let $\rho(x,y)$ be the kernel of a positive self-adjoint trace class operator $\rho \in \mathfrak{S}_1(L^2(\mathbb{R}^3))$ and $n(x) \equiv \rho(x,x)$ the corresponding density. Then for $p \in [1,\infty)$ the following estimate holds*

$$\|n\|_{L^q(\mathbb{R}^3)} \leq C_p \, \|\rho\|^{\theta}_{\mathfrak{S}_p(L^2(\mathbb{R}^3))} \, (\mathrm{tr}\, |\nabla|\rho)^{1-\theta}, \tag{3.2.1}$$

where

$$q = \frac{4p-3}{3p-2}, \qquad \theta = \frac{p}{4p-3}.$$

Proof. For the proof we proceed analogously to [19]. Since the case $p = 1$ is immediate we consider only $p > 1$. We start by considering the operator $|\nabla| - \beta n^\alpha$ where $\beta > 0$ and $\alpha > 0$ are some constants to be chosen later on. Let $\mu_1 \leq \mu_2 \leq \dots$ be the negative eigenvalues of the operator $|\nabla| - \beta n^\alpha$ and let $\{\varphi_k\}_{k\in\mathbb{N}}$ be a finite or countable collection of the corresponding ortho-normed eigenvectors. We consequently obtain

$$\mathrm{tr}\, (|\nabla| - \beta n^\alpha)\rho \geq \sum_{k\in\mathbb{N}} \langle (|\nabla| - \beta n^\alpha)\rho\, \varphi_k, \varphi_k\rangle = \sum_{j,k\in\mathbb{N}} |p_{jk}|^2 \mu_k \lambda_j,$$

where $p_{jk} = \int_{\mathbb{R}^3} \psi_j \overline{\varphi}_k$. Since $\mu_k = -|\mu_k|, \forall\, k \in \mathbb{N}$, we can rearrange this inequality in the following form

$$\operatorname{tr} \beta n^\alpha \rho = \beta \int_{\mathbb{R}^3} n^{\alpha+1} \mathrm{d}x \leq \operatorname{tr} |\nabla| \rho + \sum_{j,k \in \mathbb{N}} |p_{jk}|^2 |\mu_k| \lambda_j.$$

Now, using Hölder's inequality, and the fact that $\sum_j |p_{jk}|^2 = 1$, as well as $\sum_k |p_{jk}|^2 \leq 1$, we obtain

$$\begin{aligned}
\beta \int_{\mathbb{R}^3} n^{\alpha+1} \mathrm{d}x &\leq \operatorname{tr} |\nabla| \rho + \|\rho\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))} \left(\sum_{j \in \mathbb{N}} |\mu_j|^{p'} \right)^{1/p'} \\
&\leq \operatorname{tr} |\nabla| \rho + \|\rho\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))} C_p \left(\int_{\mathbb{R}^3} (\beta n^\alpha)^{3+p'} \mathrm{d}x \right)^{1/p'}.
\end{aligned}$$

Here the second inequality is obtained from Theorem 2.1 in [4], which states that for all $\delta > 0$

$$\sum_{j \geq 1} |\mu_j|^\delta \leq C_{\delta,d} \int_{\mathbb{R}^d} W(x)_+^{\delta+d} \mathrm{d}x,$$

where μ_j are the negative eigenvalues of the operator $|\nabla| - W$. Now with the choice $\alpha = (p-1)/(3p-2)$, setting $\alpha + 1 = q$ and

$$\beta = \left(\frac{\left(\int_{\mathbb{R}^3} n^q \mathrm{d}x \right)^{1/p}}{2C \|\rho\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))}} \right)^{p'/3},$$

it is easy to conclude

$$\left(\int_{\mathbb{R}^3} n^q \mathrm{d}x \right)^{1/q} \leq C_p \|\rho^\varepsilon\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))}^\theta \left(\operatorname{tr} |\nabla| \rho \right)^{1-\theta}.$$

□

Remark 3.2.2. The proof can easily be generalized to the d-dimensional case, where one finds

$$q = \frac{d(p-1)+p}{d(p-1)+1}, \qquad \theta = \frac{p}{d(p-1)+p}.$$

3.2.2 Local/Global-in-time existence

Before we state existence results for the Hartree system (3.1.2), we need to make appropriate uniform boundedness assumptions on the initial data. Within this work we will assume that

$$\sup_{\varepsilon \in (0,\varepsilon_0]} \left(\operatorname{tr} \rho_0^\varepsilon + \frac{1}{\varepsilon^3} \operatorname{tr} (\rho_0^\varepsilon)^2 + \operatorname{tr} \sqrt{-\varepsilon^2 \Delta + 1}\, \rho_0^\varepsilon \right) < \infty. \tag{A}$$

In the gravitational case $\kappa = -1$ we additionally assume

$$\frac{1}{\varepsilon^3} \operatorname{tr} (\rho_0^\varepsilon)^2 < \frac{C_*}{\operatorname{tr} \rho_0^\varepsilon}, \tag{B}$$

where $C_* > 0$ is a fixed, ε-independent constant to be computed in the proof of Lemma 3.2.4. To get more insight on Assumption (A) we again use the decomposition

$$\rho_0^\varepsilon = \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon \, \psi_j^\varepsilon(x) \overline{\psi_j^\varepsilon}(y),$$

to obtain

$$\operatorname{tr} \rho_0^\varepsilon = \sum_{j\in\mathbb{N}} \lambda_j^\varepsilon, \quad \operatorname{tr} (\rho_0^\varepsilon)^2 = \sum_{j\in\mathbb{N}} (\lambda_j^\varepsilon)^2.$$

We remark that $\operatorname{tr} \rho_0^\varepsilon$ is the total charge or mass of the particle system. Thus Assumption (A) implies a uniform (in ε) bound on the total charge/mass and simultaneously requires $\sum_{j\in\mathbb{N}} (\lambda_j^\varepsilon)^2 \simeq \varepsilon^3$, as $\varepsilon \to 0$. (For a construction of a density matrix ρ_0^ε, which satisfies this requirements for $\psi_j \in H^1(\mathbb{R}^3)$ we refer to [20].) This condition is to be expected from earlier papers [19, 20] and prevents us from establishing our result in the case of pure initial states, i.e. $\rho_0^\varepsilon = \psi_j^\varepsilon(x)\overline{\psi_j^\varepsilon}(y)$, or even finite combinations of pure states. Roughly speaking, the requirement of a totally mixed initial state is needed to ensure that the limiting particle density $n(t, x)$ is not too singular (bounded in $L^p(\mathbb{R}^3)$ for some $p > 1$) and thus can be successfully convolved with the Poisson kernel $\propto 1/|x|$, see (3.2.11) and (3.3.2). This is not clear a-priori as the limiting $f(t, x, \xi)$, and thus also the limiting density $n(t, x)$, in general is only a measure which does not guarantee the non-singularity with respect to Lebesgue measure. In the case of a fully mixed state though we gain a bit more regularity, which is needed in passing to the limit $\varepsilon \to 0$. Note that for any Hilbert-Schmidt $\rho^\varepsilon \in \mathfrak{S}_2(L^2(\mathbb{R}^3))$, it holds

$$\|\rho^\varepsilon\|^2_{\mathfrak{S}_2(L^2(\mathbb{R}^3))} = \operatorname{tr}(\rho^\varepsilon)^2 = \|\rho^\varepsilon(\cdot,\cdot)\|^2_{L^2(\mathbb{R}^3_x \times \mathbb{R}^3_y)} < \infty\,,$$

cf. [30]. Having in mind the scaling property (3.1.8), Assumption (A) therefore implies for the initial Wigner function $\|f^\varepsilon(0,\cdot,\cdot)\|_{L^2} < \infty$, uniformly in ε. This property is shown to be conserved by the time-evolution below and thus, yields an important uniform bound on $f^\varepsilon(t, x, \xi)$. Assumption (B), needed in the gravitational case, then additionally requires that the L^2-norm of the initial Wigner function or the total charge/mass is sufficiently small (and not only bounded), cf. Remark 3.2.5 below.

Note that the conservation laws (3.2.2) together with Assumption (A) directly imply that, for all $\varepsilon \in (0, \varepsilon_0]$, it holds

$$\|n^\varepsilon(t)\|_{L^1(\mathbb{R}^3)} = \|n^\varepsilon(0)\|_{L^1(\mathbb{R}^3)} < \infty,$$

and

$$\|f^\varepsilon(t)\|_{L^2(\mathbb{R}^3_x\times\mathbb{R}^3_\xi)} = \|f^\varepsilon(0)\|_{L^2(\mathbb{R}^3_x\times\mathbb{R}^3_\xi)} < \infty,$$

for all $t \in [0, T)$.

Now we can state the existence results:

Lemma 3.2.3. *Let ρ_0^ε be such that Assumption* (A) *holds. Then there exists a $T > 0$ and unique mild solution $\rho^\varepsilon \in C([0,T); \mathfrak{S}_1(L^2(\mathbb{R}^3))$ to* (3.1.1)*, or equivalently $\psi_k \in C^0([0,T); H_\varepsilon^{1/2}(\mathbb{R}^3)) \cap C^1([0,T); H_\varepsilon^{-1/2}(\mathbb{R}^3))$ to* (3.1.2)*, which satisfies the following conservation laws:*

$$\operatorname{tr}\rho^\varepsilon(t) = \operatorname{tr}\rho_0^\varepsilon, \quad \operatorname{tr}(\rho^\varepsilon(t))^2 = \operatorname{tr}(\rho_0^\varepsilon)^2. \tag{3.2.2}$$

Here the ε-scaled energy space $H_\varepsilon^{1/2}(\mathbb{R}^3)$ is the Sobolev space equipped with the norm

$$\|\phi_k\|^2_{H_\varepsilon^{1/2}(\mathbb{R}^3)} = \|\phi_k\|^2_{L^2(\mathbb{R}^3)} + \|(-\varepsilon^2\Delta)^{1/4}\phi_k\|^2_{L^2(\mathbb{R}^3)}. \tag{3.2.3}$$

Proof. For the existence of a unique solution we will follow the lines of [11] (where the pure state is treated) and of [6] (where a proof for density matrices with finite rank is sketched). To prove local-in-time existence we first fix ε and denote the vector $\Psi^\varepsilon = (\psi_1^\varepsilon, \psi_2^\varepsilon, \ldots)$, and likewise, Φ^ε. Then the initial-value problem for (3.1.2) can be written in a vector form as follows:

$$\begin{cases} i\varepsilon\partial_t\Psi^\varepsilon = \sqrt{-\varepsilon^2\Delta + 1}\ \Psi^\varepsilon + \kappa\mathbf{F}(\Psi^\varepsilon) \\ \Psi^\varepsilon(0) = \Phi^\varepsilon \in \boldsymbol{H}_\varepsilon^{1/2}, \quad 0 \le t < T, \end{cases} \tag{3.2.4}$$

with the nonlinearity $\mathbf{F} = (F_1, F_2, \ldots)$ given as

$$F_k(\Psi^\varepsilon) = -\left(\frac{1}{4\pi|x|} * n_{\Psi^\varepsilon}\right)\psi_k, \quad n_{\Psi^\varepsilon} = \sum_j \lambda_j^\varepsilon |\psi_j^\varepsilon|^2$$

Here

$$\boldsymbol{H}_\varepsilon^{1/2} = \left(H_\varepsilon^{1/2}(\mathbb{R}^3)\right)^{\times\infty}$$

is the ∞-fold cartesian product of the ε-scaled energy space $H_\varepsilon^{1/2}$, equipped with the norm

$$\|\Phi\|^2_{\boldsymbol{H}_\varepsilon^{1/2}} = \sum_k \lambda_k^\varepsilon \|\phi_k\|^2_{H_\varepsilon^{1/2}(\mathbb{R}^3)}.$$

We consider the integral equation

$$\psi_k^\varepsilon(t) = e^{-it\sqrt{-\varepsilon^2\Delta+1}}\phi_k^\varepsilon - i\int_0^t e^{-i(t-s)\sqrt{-\varepsilon^2\Delta+1}} F_k(\Psi^\varepsilon(s))\mathrm{d}s.$$

We are to prove that $\psi_k^\varepsilon(t)$ belongs to the Banach space $C^0([0,T); H_\varepsilon^{1/2})$ with some $T > 0$ and norm $\sup_{t\in[0,T)} \|\psi_k^\varepsilon\|_{H_\varepsilon^{1/2}}$. The proof is now organized in two steps as follows:

Step 1. $\mathbf{F}(\Psi^\varepsilon)$ *is locally Lipschitz continuous from* $\boldsymbol{H}_\varepsilon^{1/2}$ *into itself:*

This is the main point of the local-in-time existence argument. In the end we are to show that, for all $\Psi^\varepsilon, \Phi^\varepsilon \in \boldsymbol{H}_\varepsilon^{1/2}$,

$$\|\mathbf{F}(\Psi^\varepsilon) - \mathbf{F}(\Phi^\varepsilon)\|^2_{\boldsymbol{H}_\varepsilon^{1/2}} \leq C_\varepsilon(\|\Psi^\varepsilon\|^2_{\boldsymbol{H}_\varepsilon^{1/2}} + \|\Phi^\varepsilon\|^2_{\boldsymbol{H}_\varepsilon^{1/2}})^2 \, \|\Psi^\varepsilon - \Phi^\varepsilon\|^2_{\boldsymbol{H}_\varepsilon^{1/2}} \, .$$

For the convenience of the notation we introduce

$$D_\varepsilon^{1/2} := (-\varepsilon^2 \Delta)^{1/4}.$$

And by (3.2.3) it is sufficient to estimate the quantities

$$I := \|\mathbf{F}(\Psi^\varepsilon) - \mathbf{F}(\Phi^\varepsilon)\|^2_{\boldsymbol{L}^2} \qquad II := \|D_\varepsilon^{1/2}(\mathbf{F}(\Psi^\varepsilon) - \mathbf{F}(\Phi^\varepsilon))\|^2_{\boldsymbol{L}^2}.$$

In both cases, I and II, we will use the identity

$$\begin{aligned} F_k(\Psi^\varepsilon) - F_k(\Phi^\varepsilon) =& \frac{1}{2}\left(\left(\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} - n_{\Phi^\varepsilon})\right)(\psi_k^\varepsilon + \phi_k^\varepsilon)\right. \\ &\left. + \left(\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} + n_{\Phi^\varepsilon})\right)(\psi_k^\varepsilon - \phi_k^\varepsilon)\right), \end{aligned}$$

which leads, for the term I,

$$\begin{aligned} \|F_k(\Psi^\varepsilon) - F_k(\Phi^\varepsilon)\|^2_{L^2} \leq& \left\|\left(\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} - n_{\Phi^\varepsilon})\right)(\psi_k^\varepsilon + \phi_k^\varepsilon)\right\|^2_{L^2} \\ &+ \left\|\left(\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} + n_{\Phi^\varepsilon})\right)(\psi_k^\varepsilon - \phi_k^\varepsilon)\right\|^2_{L^2} \\ \leq& \left\|\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} - n_{\Phi^\varepsilon})\right\|^2_{L^6} \|\psi_k^\varepsilon + \phi_k^\varepsilon\|^2_{L^3} \\ &+ \left\|\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} + n_{\Phi^\varepsilon})\right\|^2_{\infty} \|\psi_k^\varepsilon - \phi_k^\varepsilon\|^2_{L^2} \, . \end{aligned} \tag{3.2.5}$$

Above and in the rest of the proof we use the (generalized) Minkowski and Hölder's inequalities several times tacitly. Observing that $|x|^{-1} \in L^3_w$ holds, the first term on the right-hand side of (3.2.5) can be bounded due to the generalized (or weak) Young inequality as follows

$$
\begin{aligned}
\left\|\frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} - n_{\Phi^\varepsilon})\right\|_{L^6}^2 \leq & C \left\|\frac{1}{4\pi|x|}\right\|_{L^3_w}^2 \left\|(n_{\Psi^\varepsilon} - n_{\Phi^\varepsilon})\right\|_{L^{6/5}}^2 \\
& \leq C\Big(\sum_j \lambda_j^\varepsilon \left\||\psi_j^\varepsilon|^2 - |\phi_j^\varepsilon|^2\right\|_{L^{6/5}}\Big)^2 \\
& \leq C\Big(\sum_j \lambda_j^\varepsilon \left\|\psi_j^\varepsilon + \phi_j^\varepsilon\right\|_{L^3} \left\|\psi_j^\varepsilon - \phi_j^\varepsilon\right\|_{L^2}\Big)^2 \\
& \leq C \sum_j \lambda_j^\varepsilon \left\|\psi_j^\varepsilon + \phi_j^\varepsilon\right\|_{L^3}^2 \sum_l \lambda_l^\varepsilon \left\|\psi_l^\varepsilon - \phi_l^\varepsilon\right\|_{L^2}^2 \\
& \leq C \sum_j \lambda_j^\varepsilon \left\|\psi_j^\varepsilon + \phi_j^\varepsilon\right\|_{H^{1/2}}^2 \sum_l \lambda_l^\varepsilon \left\|\psi_l^\varepsilon - \phi_l^\varepsilon\right\|_{L^2}^2 \\
& \leq C_\varepsilon(\|\Psi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 + \|\Phi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2) \|\Psi^\varepsilon - \Phi^\varepsilon\|_{\boldsymbol{L}^2}^2
\end{aligned}
\tag{3.2.6}
$$

where we use the Sobolev inequality $\|u\|_{L^3} \leq C\|u\|_{H^{1/2}}$ and the fact that $\|u\|_{H^{1/2}} \leq \frac{1}{\varepsilon}\|u\|_{H_\varepsilon^{1/2}}$. By abuse of notation, only in this proof, we denote all the constants that might appear, the same, namely C. Although it would not make a difference for it is fixed, here and in the sequel of this proof we emphasize the ε dependence of the constants by a subscript just to distinguish it from the uniform bounds which we will commonly use afterwards.

The second term in (3.2.5) can be estimated using the operator inequality $|x-y|^{-1} \leq \frac{\pi}{2}(-\Delta_{x-y})^{1/2}$ (see, e.g., [15]) and translational invariance, i.e., we use that $\Delta_{x-y} = \Delta_x$ holds for all $y \in \mathbb{R}^3$:

$$
\begin{aligned}
\left\|\frac{1}{4\pi|x|} * n_{\Psi^\varepsilon}\right\|_\infty & \leq \sum_j \lambda_j^\varepsilon \sup_{y\in\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\psi_j^\varepsilon|^2}{|x-y|} \mathrm{d}x \\
& \leq \sum_j \lambda_j^\varepsilon \left\|(-\Delta)^{1/4}\psi_j^\varepsilon\right\|_{L^2}^2 \leq C_\varepsilon \sum_j \lambda_j^\varepsilon \left\|D_\varepsilon^{1/2}\psi_j^\varepsilon\right\|_{L^2}^2 .
\end{aligned}
\tag{3.2.7}
$$

A similar estimate holds for the term with n_{Φ^ε}. Now combining (3.2.6) and (3.2.7) we find that

$$
\begin{aligned}
I \leq & \sum_k \lambda_k^\varepsilon \|F_k(\Psi^\varepsilon) - F_k(\Phi^\varepsilon)\|_{L^2}^2 \\
& \leq C_\varepsilon(\|\Psi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 + \|\Phi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2)^2 \sum_k \lambda_k^\varepsilon \|\psi_k + \phi_k\|_{L^3}^2 \|\Psi^\varepsilon - \Phi^\varepsilon\|_{\boldsymbol{L}^2}^2 \\
& \qquad + C_\varepsilon(\|\Psi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 + \|\Phi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2)^2 \sum_k \lambda_k^\varepsilon \|(\psi_k - \phi_k)\|_{L^2}^2 \\
& \leq C_\varepsilon(\|\Psi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 + \|\Phi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2)^2 \|\Psi^\varepsilon - \Phi^\varepsilon\|_{\boldsymbol{H}^{1/2}}^2 .
\end{aligned}
$$

Now, it remains to estimate II. To this end, we appeal to the generalized (or fractional) Leibniz rule (see, e.g., [11] and references therein) which leads

$$\begin{aligned}
\left\|D_\varepsilon^{1/2}(F_k(\Psi^\varepsilon)-F_k(\Phi^\varepsilon))\right\|_{L^2}^2 \le& \left\|D_\varepsilon^{1/2}\left(\left(\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon})\right)(\psi_k+\phi_k)\right)\right\|_{L^2}^2 \\
&+\left\|D_\varepsilon^{1/2}\left(\left(\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}+n_{\Phi^\varepsilon})\right)(\psi_k-\phi_k)\right)\right\|_{L^2}^2 \\
\le& \left\|D_\varepsilon^{1/2}\left(\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon})\right)\right\|_{L^6}^2\left\|\psi_k+\phi_k\right\|_{L^3}^2 \\
&+\left\|\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon})\right\|_{\infty}^2\left\|D_\varepsilon^{1/2}(\psi_k+\phi_k)\right\|_{L^2}^2 \\
&+\left\|D_\varepsilon^{1/2}\left(\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}+n_{\Phi^\varepsilon})\right)\right\|_{L^6}^2\left\|\psi_k-\phi_k\right\|_{L^3}^2 \\
&+\left\|\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}+n_{\Phi^\varepsilon})\right\|_{\infty}^2\left\|D_\varepsilon^{1/2}(\psi_k-\phi_k)\right\|_{L^2}^2 .
\end{aligned} \tag{3.2.8}$$

Before we proceed, we recall some facts from [27], Section V.3.1. For $0<\alpha<3$, the potential operator $D^{-\alpha}=(-\Delta)^{-\alpha/2}$ corresponds to $f\mapsto G_\alpha * f$, with $f\in\mathcal{S}(\mathbb{R}^3)$, and we have that

$$G_\alpha(x)=\frac{c_\alpha}{|x|^{3-\alpha}}\in L^{3/(3-\alpha)_w}(\mathbb{R}^3)\quad\text{for}\quad 0<\alpha<3.$$

Thus regarding the equality $D^{-2}f=\frac{1}{4\pi|x|}*f$, the first term on the right-hand side of (3.2.8) is found to be

$$\begin{aligned}
\left\|D_\varepsilon^{1/2}\left(\frac{1}{4\pi|x|}*(n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon})\right)\right\|_{L^6}^2 &\le C_\varepsilon\left\|D^{-3/2}(n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon})\right\|_{L^6}^2 \\
&\le C_\varepsilon\left\|G_{3/2}*(n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon})\right\|_{L^6}^2 \\
&\le C_\varepsilon\left\|G_{3/2}\right\|_{L^2_w}^2\left\|n_{\Psi^\varepsilon}-n_{\Phi^\varepsilon}\right\|_{L^{3/2}}^2 \\
&\le C_\varepsilon\sum_j\lambda_j^\varepsilon\left\|\psi_j^\varepsilon+\phi_j^\varepsilon\right\|_{L^3}^2\sum_l\lambda_l^\varepsilon\left\|\psi_l^\varepsilon-\phi_l^\varepsilon\right\|_{L^3}^2 \\
&\le C_\varepsilon\sum_j\lambda_j^\varepsilon\left\|\psi_j^\varepsilon+\phi_j^\varepsilon\right\|_{L^3}^2\sum_l\lambda_l^\varepsilon\left\|\psi_l^\varepsilon-\phi_l^\varepsilon\right\|_{H^{1/2}}^2 \\
&\le C_\varepsilon\left\|\Psi^\varepsilon+\Phi^\varepsilon\right\|_{\boldsymbol{L}^3}^2\left\|\Psi^\varepsilon-\Phi^\varepsilon\right\|_{\boldsymbol{L}^2}^2
\end{aligned}$$

Here we employ same arguments as in (3.2.6). Now the ∞-norm occurring in the second term in (3.2.8) can be estimated by using the (3.2.7) once more:

$$\begin{aligned}
\left\| \frac{1}{4\pi|x|} * (n_{\Psi^\varepsilon} - n_{\Phi^\varepsilon}) \right\|_\infty^2 \leq & \left(\sum_j \lambda_j^\varepsilon \sup_{y\in\mathbb{R}^3} \left| \int_{\mathbb{R}^3} \frac{|\psi_j^\varepsilon|^2 - |\phi_j^\varepsilon|^2}{|x-y|} \mathrm{d}x \right| \right)^2 \\
\leq & \left(\sum_j \lambda_j^\varepsilon \sup_{y\in\mathbb{R}^3} |\langle \psi_j^\varepsilon + \phi_j^\varepsilon, \frac{1}{|x-y|} \psi_j^\varepsilon - \phi_j^\varepsilon \rangle| \right)^2 \\
\leq & \left(\sum_j \lambda_j^\varepsilon \left\| (-\Delta)^{1/4} (\psi_j^\varepsilon - \phi_j^\varepsilon) \right\|_{L^2} \left\| (-\Delta)^{1/4} (\psi_j^\varepsilon - \phi_j^\varepsilon) \right\|_{L^2} \right)^2 \\
\leq & C_\varepsilon \left\| \Psi^\varepsilon + \Phi^\varepsilon \right\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 \left\| \Psi^\varepsilon - \Phi^\varepsilon \right\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 .
\end{aligned} \tag{3.2.9}$$

The remaining terms in (3.2.8) deserve no further comment since they can be estimated in a similar fashion to all estimates obtained so far. Thus, for each fixed ε we conclude that

$$\|\mathbf{F}(\Psi^\varepsilon) - \mathbf{F}(\Phi^\varepsilon)\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 \leq C_\varepsilon (\|\Psi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2 + \|\Phi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2)^2 \|\Psi^\varepsilon - \Phi^\varepsilon\|_{\boldsymbol{H}_\varepsilon^{1/2}}^2$$

and the proof of the claim of the *Step 1* is complete.

Step 2. Conclusion:
Returning to the proof of Lemma 3.2.3, we note that $\sqrt{-\varepsilon^2\Delta + 1}$ gives rise to a self-adjoint operator and generates C^0-semigroup acting on $H_\varepsilon^{1/2}$, i.e.,

$$\left\{ e^{-it\sqrt{-\varepsilon^2\Delta+1}} \right\}_{t\in\mathbb{R}} \quad : \quad H_\varepsilon^{1/2} \to H_\varepsilon^{-1/2}.$$

Local-wellposedness follows by standard methods for evolution equations with locally Lipschitz nonlinearities. That is, existence and uniqueness of a solution $\Psi^\varepsilon \in C([0,T); \boldsymbol{H}_\varepsilon^{1/2})$ is deduced by a fixed point argument, for $T > 0$ sufficiently small, as well as the blow up alternative (see [23] for general theory on semilinear evolution equations). Finally, note that $\psi_k^\varepsilon \in C^1([0,T); H_\varepsilon^{-1/2})$ follows by the equation (3.1.2) itself.

To be able to accomplish the proof of Lemma 3.2.3, it only remained to prove the conservation laws (3.2.2). Conservation of charge/mass can easily be obtained by multiplying (3.1.2) by $i\lambda_j^\varepsilon \overline{\psi_j^\varepsilon}$ and integrating over $\mathbb{R}^3$ after summation on $j \in \mathbb{N}$. The real part gives the conservation law. Or in the Heisenberg picture, one can simply take the trace of the equation (3.1.1) which leads conservation law:

$$\frac{\mathrm{d}}{\mathrm{d}t} \operatorname{tr} \rho^\varepsilon = 0$$

For the conservation of the Hilbert-Schmidt norm, we multiply the equation (3.1.1) by $\overline{\rho^\varepsilon}$ then take the trace by recalling the fact from [2] that, for $A, B \in \mathfrak{S}_2$, i.e., Hilbert-Schmidt operator, we have

$$\operatorname{tr} AB = \int_{\mathbb{R}^6} a(x,z) b(z,x) \mathrm{d}z \mathrm{d}x$$

where a and b are the corresponding kernels of the operators A and B, respectively. After simple calculation, one obtains

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \operatorname{tr}(\rho^\varepsilon)^2 = 0$$

This completes the proof. $\square$

Lemma 3.2.4. *The solution stated above exists globally in-time, i.e.* $T = \infty$, *and we additionally have conservation of energy:* $\mathcal{E}_{\mathrm{H}}^\varepsilon(t) = \mathcal{E}_{\mathrm{H}}^\varepsilon(0)$, *provided that one of the following conditions is satisfied:*

i) $\kappa = 1$,

ii) $\kappa = -1$ *and Assumption* (B) *is satisfied.*

In particular we have the following uniform bound

$$\mathcal{E}_{\mathrm{kin}}^\varepsilon(t) \leq C, \quad \forall\, t \in [0, \infty). \tag{3.2.10}$$

Proof. Formally, for the conservation of energy we multiply (3.1.2) by $\lambda_j^\varepsilon \overline{\dot{\psi}_j^\varepsilon} \in H_\varepsilon^{-1/2}$ then sum over $j \in \mathbb{N}$ and integrate over $\mathbb{R}^3$:

$$\begin{aligned} i\varepsilon \sum_j \lambda_j^\varepsilon \int_{\mathbb{R}^3} |\dot{\psi}_j^\varepsilon|^2 \mathrm{d}x =& \sum_j \lambda_j^\varepsilon \int_{\mathbb{R}^3} \frac{\mathrm{d}}{\mathrm{d}t} (\frac{1}{2} |(-\varepsilon^2 \Delta + 1)^{1/4} \psi_j^\varepsilon|^2) \mathrm{d}x \\ &+ \frac{\kappa}{4\pi} \int_{\mathbb{R}^6} \frac{n^\varepsilon(t,y)}{|x-y|} \frac{\mathrm{d}}{\mathrm{d}t} (\frac{1}{2} n^\varepsilon(t,x)) \mathrm{d}y \mathrm{d}x \\ =& \frac{\mathrm{d}}{\mathrm{d}t} \frac{1}{2} \sum_j \lambda_j^\varepsilon \|(-\varepsilon^2 \Delta + 1)^{1/4} \psi_j^\varepsilon\|_{L^2(\mathbb{R}^3)}^2 \\ &+ \frac{\mathrm{d}}{\mathrm{d}t} \frac{\kappa}{16\pi} \int_{\mathbb{R}^6} \frac{n^\varepsilon(t,y) n^\varepsilon(t,x)}{|x-y|} \mathrm{d}y \mathrm{d}x. \end{aligned}$$

Real part on the right-hand side gives the desired conservation law. This computation is formal since the pairing of two elements of $H_\varepsilon^{-1/2}$ is not well-defined. However, by introducing a regularization procedure as in [11] the proof of the energy conservation can be made rigorous. This is out of the scope of the present work.

In order to obtain the uniform a-priori bound (3.2.10) we shall use (3.2.1), with $p = 2$, which yields

$$\begin{aligned}\|n^\varepsilon(t)\|_{L^{5/4}} &\le C_2 \|\rho^\varepsilon(t,\cdot,\cdot)\|_{L^2}^{2/5} (\operatorname{tr}|\nabla|\rho^\varepsilon(t))^{3/5} \\ &\le C_2\, \varepsilon^{-3/5} \|\rho^\varepsilon(0,\cdot,\cdot)\|_{L^2}^{2/5} \left(\operatorname{tr}\sqrt{-\varepsilon^2\Delta+1}\;\rho^\varepsilon(t)\right)^{3/5},\end{aligned} \tag{3.2.11}$$

due to the second conservation law in (3.2.2) and the fact that $\varepsilon|\nabla| \le \sqrt{-\varepsilon^2\Delta+1}$, as can be seen on the level of the Fourier-symbols. On the other hand, recalling the Sobolev inequality

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{n^\varepsilon(t,x)n^\varepsilon(t,y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y \le C_\mathrm{s}\|n^\varepsilon(t)\|_{L^{6/5}}^2,$$

and interpolating the density via $\|n^\varepsilon(t)\|_{L^{6/5}} \le \|n^\varepsilon(t)\|_{L^1}^{1/6}\,\|n^\varepsilon(t)\|_{L^{5/4}}^{5/6}$, we obtain

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{n^\varepsilon(t,x)n^\varepsilon(t,y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y \le \tilde{C}\mathcal{E}^\varepsilon_{\mathrm{kin}}(t), \quad \forall\, t\in[0,\infty),$$

where $\tilde{C} = C_\mathrm{s} C_2^{5/3}(\operatorname{tr}\rho_0^\varepsilon)^{1/3}\|f^\varepsilon(0,\cdot,\cdot)\|_{L^2}^{2/3}$ is ε-independent by Assumption (A). On the one hand, this shows that the initial energy is indeed well defined and uniformly bounded in ε for both $\kappa = \pm 1$. Moreover, we immediately conclude the uniform boundedness of the kinetic energy in the case $\kappa = 1$ and hence, global-in-time existence of solutions. In the case $\kappa = -1$ we only get, from energy conservation, that

$$\mathcal{E}^\varepsilon_\mathrm{H}(0) = \mathcal{E}^\varepsilon_{\mathrm{kin}}(t) - \frac{1}{8\pi}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{n^\varepsilon(t,x)n^\varepsilon(t,y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y \ge \left(1-\frac{\tilde{C}}{8\pi}\right)\mathcal{E}^\varepsilon_{\mathrm{kin}}(t).$$

Uniform boundedness of $\mathcal{E}^\varepsilon_{\mathrm{kin}}(t)$, and hence, global-in-time existence, can therefore be concluded if $\tilde{C} < 8\pi$, which holds true under Assumption (B). ☐

Remark 3.2.5. In comparison to the proof given in [11] we needed to invoke slightly different arguments in order to obtain the uniform (w.r.t. ε) bound (3.2.10). The requirement $\tilde{C} < 8\pi$ directly leads to Assumption (B) with $C_* = \frac{(8\pi)^3}{C_\mathrm{s}^3 C_2^5}$. Note however, that in our mixed-state case we can no longer characterize the condition $\tilde{C} < 8\pi$ by the solution of the corresponding single-state ground state problem as it is done in [11].

3.2.3 Compactness argument

We close this section by giving the appropriate compactness argument that is going to be used in the following section in which the convergence results are shown. The following lemma is an adaptation of Lemma C.1 in [18] that has been stated and proven in [1]. Nevertheless, we state it with its proof.

Lemma 3.2.6. *Let X be a separable Banach space, X' the dual space and $X'-w*$ the dual equipped with the weak-$*$ topology. If $(f_n)_{n\in\mathbb{N}} \subset C([0,\tau]; X'-w*)$ is a sequence of functions such that*

(i) *(uniform boundedness)* $\exists C > 0$ *such that* $\sup_{n\in\mathbb{N}} \|f_n(t)\|_{L^\infty([0,\tau];X')} < C$

(ii) *(time equicontinuity)* $\forall \phi \in X$, *the sequence of functions* $t \mapsto \langle f_n(t), \phi\rangle_{X'\times X}$ *is uniformly continuous in* $t \in [0,\tau]$, *uniformly in* $n \in \mathbb{N}$.

Then $(f_n)_{n\in\mathbb{N}}$ is relatively compact in $C([0,\tau]; X'-w*)$, i.e. there exists $f \in C([0,\tau]; X'-w*)$ and a subsequence satisfying

$$\forall \phi \in X, \qquad \langle f_n(t), \phi\rangle \longrightarrow \langle f(t), \phi\rangle \qquad \textit{for} \quad n \to \infty.$$

Lemma 3.2.6 has been applied in Section 3.3 to the pair $(X', X) = (\mathcal{S}', \mathcal{S})$ and $(X', X) = (\mathcal{M}, C_0)$.

Proof. Banach$-$Alaoglu theorem asserts that the closed unit ball of the dual space of a separable normed vector space is sequentially compact in the weak-$*$ topology. In fact, the weak-$*$ topology on the closed unit ball of the dual of a separable space is metrizable. To see this, let B_R be the closed unit ball in X'. Since X is separable, let $(\phi_k)_{k\geq 1}$ be a countable dense subset in X. Then the following defines a metric for $f, g \in B_R$

$$d(f,g) = \sum_{k\geq 1} 2^{-k} \frac{|\langle f-g, \phi_k\rangle_{X'\times X}|}{1 + |\langle f-g, \phi_k\rangle_{X'\times X}|}.$$

Thus compactness and sequential compactness are equivalent. Hence, for each t fixed, the sequence $f_n(t)$ is relatively and sequentially compact in $X'-w*$. Since we have the uniform boundedness of the sequence $f_n(t)$ from (i), to be able to apply Arzelà-Ascoli lemma, it remains to show the equicontinuity, that is

$$\sup_{n\in\mathbb{N}} d(f_n(t), f_n(s)) \longrightarrow 0 \qquad \text{as} \qquad |t-s| \to 0, \quad t,s \in [0,\tau].$$

For fixed $h > 0$, we have

$$d(f_n(t), f_n(s)) \leq \sup_{1\leq k\leq h} \sup_{n\in\mathbb{N}} |\langle f_n(t) - g_n(t), \phi_k\rangle_{X'\times X}| + \frac{1}{2^h}.$$

The first term on the right-hand side goes to the zero as $t \to s$ which is exactly what the hypothesis (ii) says:

$$\sup_{n\in\mathbb{N}} |\langle f_n(t) - g_n(t), \phi_k\rangle_{X'\times X}| \longrightarrow 0 \qquad \text{as} \qquad |t-s| \to 0.$$

This concludes the proof by observing that the second term is arbitrarily small as $h \to \infty$. $\square$

3.3 Classical limit

The main result of this chapter is as follows:

Theorem 2. *Let $\varepsilon_0 < 1$ and assume that the initial data $\rho_0^\varepsilon \in \mathfrak{S}_1(L^2(\mathbb{R}^3))$ is a density matrix operator, such that* (A) *holds. In the gravitational case $\kappa = -1$ we additionally assume* (B) *holds true where $C_* > 0$ is a fixed ε-independent constant computed in the Lemma 3.2.4.*

Then there exists a unique mild solution $\rho^\varepsilon \in C([0,\infty); \mathfrak{S}_1(L^2(\mathbb{R}^3))$ of the relativistic Hartree system (3.1.1) *and its Wigner transform $f^\varepsilon[\rho^\varepsilon] \in C([0,\infty); L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi))$ converges, up to extraction of sub-sequences,*

$$f^\varepsilon[\rho^\varepsilon] \xrightarrow{\varepsilon \to 0} f \quad in\ C([0,\tau]; \mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi) - w*),$$

for any $\tau < \infty$, where $f \in C([0,\tau]; \mathcal{M}^+(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)) \cap L^\infty([0,\tau]; L^1 \cap L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi))$ is a distributional solution of the relativistic Vlasov-Poisson system (3.1.9)*. Here $\mathcal{M}^+$ is the space of positive bounded Borel measures on phase-space, equipped with the weak-$*$ topology.*

The above given theorem shows that distributional solutions to (3.1.9) can indeed be interpreted as the classical limit (on any compact time-interval) of solutions to (3.1.2), or equivalently (3.1.1).

In the sequel, we will use the following shorthand notation for the Fourier transform with respect to ξ:

$$\hat{\varphi}(\eta) \equiv (\mathcal{F}_{\xi\to\eta}\varphi)(\eta)$$

Proof. The proof of the Theorem 2 consists of three steps:

Step 1. We first note that due to Assumption (A) and the conservation laws (3.2.2), the Wigner function $f^\varepsilon(t)$ is uniformly bounded in $L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)$ and in $\mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)$, where the later follows from Proposition 3.1.1 in Section 3.1.2. Thus, for every fixed $t \in [0,\infty)$, it holds (up to extraction of sub-sequences): $f^\varepsilon(t) \rightharpoonup f(t)$, as $\varepsilon \to 0$, in $\mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi) - w*$ and in $L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi) - w$. Moreover it has been shown in Section 2 that the limit $f \in \mathcal{M}^+(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)$, i.e. a positive phase-space measure.

Step 2. Next we shall prove the time-equicontinuity of $f^\varepsilon(t,x,\xi)$. To this end, we have to show that $\partial_t f^\varepsilon$ is bounded in $L^\infty((0,\tau), \mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi))$, for any $\tau < \infty$. We consequently consider the (phase space) weak formulation of the Wigner transformed evolution equation, i.e.

$$-\langle \partial_t f^\varepsilon, \phi\rangle = \langle \Gamma^\varepsilon f^\varepsilon, \phi\rangle + \langle \Theta^\varepsilon[V^\varepsilon] f^\varepsilon, \phi\rangle, \tag{3.3.1}$$

where $\phi \in \mathcal{S}(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)$ and we write $\langle \,\cdot\, , \,\cdot\, \rangle$ for the corresponding duality bracket on $\mathcal{S}$. Here we recall that $\Gamma^\varepsilon f^\varepsilon$ is given by

$$\Gamma^\varepsilon f^\varepsilon(t,x,\xi) = \frac{i}{(2\pi)^3} \iint_{\mathbb{R}^3\times\mathbb{R}^3} e^{iy\cdot(x-\eta)}\; y\cdot\gamma^\varepsilon(y,\xi) f^\varepsilon(t,\eta,\xi)\,\mathrm{d}y\,\mathrm{d}\eta,$$

where

$$\gamma^\varepsilon(y,\xi) := \frac{2\xi}{\sqrt{|\xi+\varepsilon\frac{y}{2}|^2+1}+\sqrt{|\xi-\varepsilon\frac{y}{2}|^2+1}} \in \mathbb{R}^3,$$

and the nonlinear potential $V^\varepsilon(t,x)$ enters via the well known operator, cf. [19, 20]

$$\Theta^\varepsilon[V^\varepsilon] f^\varepsilon(t,x,\xi) = \frac{i}{(2\pi)^3} \iint_{\mathbb{R}^3\times\mathbb{R}^3} e^{i\eta\cdot(z-\xi)} \delta^\varepsilon(t,x,\eta) f^\varepsilon(t,x,z)\,\mathrm{d}\eta\,\mathrm{d}z.$$

whose symbol is given by

$$\delta^\varepsilon(t,x,\eta) := \frac{1}{\varepsilon}\Big(V^\varepsilon(t,x+\varepsilon\frac{\eta}{2}) - V^\varepsilon(t,x-\varepsilon\frac{\eta}{2})\Big) = \eta\cdot\int_{-1/2}^{1/2} \nabla_x V^\varepsilon(t,x+\varepsilon s\eta)\,\mathrm{d}s.$$

In order to estimate the first term on the r.h.s. of (3.3.1), we use an inverse Fourier transform w.r.t. x and Plancherel's theorem to obtain

$$\begin{aligned}
|\langle \Gamma^\varepsilon f^\varepsilon, \phi\rangle| &= \Big| \iint_{\mathbb{R}^6} \Big(\int_{\mathbb{R}^3} e^{-iy\cdot\eta} (\mathcal{F}^{-1}_{x\to y} \nabla_x \phi)(y,\xi)\cdot\gamma^\varepsilon(\xi,y)\,\mathrm{d}y\Big) f^\varepsilon(t,\eta,\xi)\mathrm{d}\eta\,\mathrm{d}\xi \Big| \\
&\le \|f^\varepsilon(t)\|_{L^2} \Big(\iint_{\mathbb{R}^6} \big|(\mathcal{F}^{-1}_{x\to y}\nabla_x\phi)(y,\xi)\big|^2 \,|\gamma^\varepsilon(\xi,y)|^2\,\mathrm{d}y\,\mathrm{d}\xi\Big)^{1/2} \\
&\le \|f^\varepsilon(t)\|_{L^2} \|\nabla_x \phi\|_{L^2},
\end{aligned}$$

where the second inequality follows from the fact that $|\gamma^\varepsilon| \le 1$, for all $\varepsilon \in (0,\varepsilon_0]$. Since $f^\varepsilon(t,x,\xi)$ is uniformly bounded in $L^2(\mathbb{R}^3_x\times\mathbb{R}^3_\xi)$ for all $t\in[0,\infty)$, due to (3.2.2) and Assumption (A), we obtain the desired uniform bound for $|\langle\Gamma^\varepsilon f^\varepsilon,\phi\rangle|$. Next, we consider the nonlinear term on the r.h.s. of (3.3.1). After a Fourier transform w.r.t. ξ, we need to estimate

$$\begin{aligned}
&|\langle \Theta^\varepsilon[V^\varepsilon] f^\varepsilon, \phi\rangle| \\
&\quad = \Big| \iint_{\mathbb{R}^6} \hat\phi(x,\eta) \Big(\int_{-1/2}^{1/2} \eta\cdot\nabla_x V^\varepsilon(t,x+\varepsilon s\eta)\mathrm{d}s\Big) (\mathcal{F}^{-1}_{x\to y} f^\varepsilon)(t,x,\eta)\mathrm{d}x\,\mathrm{d}\eta\Big|.
\end{aligned}$$

Using the generalized Young inequality we have

$$\|\nabla_x V^\varepsilon(t)\|_{L^2(\mathbb{R}^3)} \le C \Big\| \nabla_x |x|^{-1} \Big\|_{L^{3/2}_w(\mathbb{R}^3)} \|n^\varepsilon(t)\|_{L^{6/5}(\mathbb{R}^3)}, \tag{3.3.2}$$

and by interpolation between $L^1(\mathbb{R}^3)$ and $L^{5/4}(\mathbb{R}^3)$, one obtains

$$\|n^\varepsilon(t)\|_{L^{6/5}} \le \|n^\varepsilon(t)\|^{1/6}_{L^1} \|n^\varepsilon(t)\|^{5/6}_{L^{5/4}} \le \mathrm{tr}(\rho^\varepsilon(t))^{1/6} \,\|f(t,\cdot,\cdot)^\varepsilon\|^{1/3}_{L^2} (\mathcal{E}^\varepsilon_{\mathrm{kin}}(t))^{1/2}.$$

Due to the conservation laws (3.2.2) and the uniform bound on the kinetic energy (3.2.10) we therefore find that $\|\nabla_x V^\varepsilon(t)\|_{L^2}$ is uniformly bounded as $\varepsilon \to 0$, for all $t \in [0,\infty)$. Thus, we can estimate

$$\begin{aligned}
&|\langle \Theta^\varepsilon[V^\varepsilon] f^\varepsilon, \phi\rangle| \\
&\quad \leq \|f^\varepsilon(t)\|_{L^2} \Big(\iint_{\mathbb{R}^6} |\hat{\phi}(x,\eta)|^2 |\eta|^2 \Big| \int_{-1/2}^{1/2} \nabla_x V^\varepsilon(t, x+\varepsilon s\eta) \mathrm{d}s \Big|^2 \mathrm{d}x\, \mathrm{d}\eta \Big)^{1/2} \\
&\quad \leq \|f^\varepsilon(t)\|_{L^2} \|\nabla_x V^\varepsilon(t)\|_{L^2} \Big(\int_{\mathbb{R}^3} \sup_{y\in\mathbb{R}^3} |\hat{\phi}(y-\varepsilon s\eta, \eta)|^2 |\eta|^2 \mathrm{d}\eta \Big)^{1/2} \\
&\quad \leq \|f^\varepsilon(t)\|_{L^2} \, \|\nabla_x V^\varepsilon(t)\|_{L^2} \, \| \sup_{y\in\mathbb{R}^3} |\hat{\phi}(y,\eta)| |\eta| \, \|_{L^2} < \infty,
\end{aligned}$$

uniformly in ε. Thus, $\partial_t f^\varepsilon$ is bounded in $L^\infty((0,\tau), \mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi))$, uniformly in ε, and we conclude that (again up to extraction of sub-sequences)

$$\begin{aligned}
f^\varepsilon \stackrel{\varepsilon\to 0}{\longrightarrow} f \qquad &\text{in} \qquad C((0,\tau); \mathcal{S}'(\mathbb{R}^3_x \times \mathbb{R}^3_\xi) - w*), \\
\text{and} \quad &\text{in} \qquad L^\infty((0,\tau); L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)) - w*.
\end{aligned}$$

Together with the results of *Step 1* this implies (by the virtue of the Lemma 3.2.6)

$$f \in C((0,\tau); \mathcal{M}^+(\mathbb{R}^3_x \times \mathbb{R}^3_\xi) - w*) \cap L^\infty((0,\tau); L^1 \cap L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)).$$

Step 3. It remains to identify the limiting $f(t,x,\xi)$, by passing to the limit in the (full) weak formulation of the Wigner transformed evolution equation, i.e.

$$\begin{aligned}
&\int_0^\infty \iint_{\mathbb{R}^6} \big(- \partial_t \sigma(t) \phi(x,\xi) - \sigma(t) \Gamma^\varepsilon \phi(x,\xi) \big) f^\varepsilon(t,x,\xi)\, \mathrm{d}x\, \mathrm{d}\xi\, \mathrm{d}t \\
&+ \int_0^\infty \iint_{\mathbb{R}^6} \sigma(t) \Theta^\varepsilon[V^\varepsilon] \phi(x,\xi) f^\varepsilon(t,x,\xi)\, \mathrm{d}x\, \mathrm{d}\xi\, \mathrm{d}t = \iint_{\mathbb{R}^6} \sigma(0) \phi(x,\xi) f_0^\varepsilon(x,\xi)\, \mathrm{d}x\, \mathrm{d}\xi,
\end{aligned} \tag{3.3.3}$$

where $\sigma \in C_0^\infty(\mathbb{R}^+_t)$ and $\phi \in \mathcal{S}(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)$. Throughout this step (where we identify the limit point), we will use the test functions $\phi \in \mathcal{S}(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)$ such that $\hat{\phi}(x,\eta)$ is compactly supported. First it is easily seen that

$$\lim_{\varepsilon\to 0} \sup_{t\in[0,\tau]} |\langle f^\varepsilon, \Gamma^\varepsilon \phi\rangle - \langle f, \nabla_x \phi \cdot \frac{\xi}{\sqrt{|\xi|^2+1}}\rangle| = 0,$$

since $f^\varepsilon \rightharpoonup f$ in $L^\infty((0,\tau]; L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi)) - w*$, as shown in *Step 2*, and the convergence of the rest of the duality bracket is strong in $C([0,\tau]; L^2(\mathbb{R}^3_x \times \mathbb{R}^3_\xi))$. Concerning the nonlinear term, we have to show

$$\lim_{\varepsilon\to 0} \sup_{t\in[0,\tau]} |\langle f^\varepsilon, \Theta^\varepsilon[V^\varepsilon]\phi\rangle - \langle f, \nabla_x V \cdot \nabla_\xi \phi\rangle| = 0. \tag{3.3.4}$$

Similarly to what is done above, after invoking a Fourier transform w.r.t. ξ, it is sufficient to prove that

$$\lim_{\varepsilon\to 0}\Big(\hat{\phi}(x,\eta)\int_{-1/2}^{1/2}\eta\cdot\nabla_x V^\varepsilon(t,x+\varepsilon s\eta)\mathrm{d}s\Big)=\hat{\phi}(x,\eta)\eta\cdot\nabla_x V(t,x),$$

in $C([0,\tau];L^2(\mathbb{R}^3_x\times\mathbb{R}^3_\xi))$ strongly. In order to do so we denote the compact support of $\hat{\phi}$ by $\Omega :\subseteq \Omega_x\times\Omega_\eta$ and write

$$\begin{aligned}
&\int_{-1/2}^{1/2}\Big(\iint_\Omega|\hat{\phi}(x,\eta)|\eta||^2|\nabla_x V^\varepsilon(t,x+\varepsilon s\eta)-\nabla_x V(t,x)|^2\mathrm{d}x\,\mathrm{d}\eta\Big)^{1/2}\mathrm{d}s\\
&\le \sup_{x,\eta\in\Omega}|\hat{\phi}(x,\eta)|\eta||\int_{-1/2}^{1/2}\Big(\iint_\Omega|\nabla_x V^\varepsilon(t,x+\varepsilon s\eta)-\nabla_x V(t,x+\varepsilon s\eta)|^2\mathrm{d}x\,\mathrm{d}\eta\\
&\qquad\qquad+\iint_\Omega|\nabla_x V(t,x+\varepsilon s\eta)-\nabla_x V(t,x)|^2\mathrm{d}x\,\mathrm{d}\eta\ \Big)^{1/2}\mathrm{d}s\\
&=: \sup_{x,\eta\in\Omega}|\hat{\phi}(x,\eta)|\eta||\int_{-1/2}^{1/2}(I^\varepsilon+J^\varepsilon)^{1/2}\,\mathrm{d}s.
\end{aligned}$$

First, we consider the term J^ε: Using Plancherel's Theorem we can write

$$\begin{aligned}
J^\varepsilon &= \iint_\Omega|\nabla_x V(t,x+\varepsilon s\eta)-\nabla_x V(t,x)|^2\mathrm{d}x\,\mathrm{d}\eta\\
&= \iint_\Omega|(\mathcal{F}_{x\to z}\nabla_x V)(t,z)|^2\,|\,e^{i\varepsilon s\eta\cdot z}-1|^2\mathrm{d}x\,\mathrm{d}\eta,
\end{aligned}$$

from which we conclude that $J^\varepsilon\to 0$, as $\varepsilon\to 0$, by dominant convergence. In order to treat the term I^ε we take into account that V^ε solves the Poisson equation

$$-\kappa\Delta V^\varepsilon = n^\varepsilon(t,x),\quad \kappa=\pm 1$$

with $n^\varepsilon(t)\in L^{5/4}(\mathbb{R}^3)\cap L^1(\mathbb{R}^3)$, uniformly in ε. Due to the regularizing property of the Poisson equation we have $\nabla_x V^\varepsilon\in W^{1,5/4}_{\mathrm{loc}}(\mathbb{R}^3)$ uniformly in ε, which is compactly embedded in $L^2_{\mathrm{loc}}(\mathbb{R}^3)$. We therefore infer that, for all $t\in[0,\tau]$, it holds

$$\nabla_x V^\varepsilon(t)\xrightarrow{\varepsilon\to 0}\nabla_x V(t)\quad\text{in}\quad L^2(\mathcal{O}),\tag{3.3.5}$$

where $\mathcal{O}=\{z:=x+\varepsilon s\eta\in\mathbb{R}^3|\ (x,\eta)\in(\Omega^3_x\times\Omega^3_\eta)\}$. We finally recall the result of Proposition 3.1.5 from Section 3.1.2 (and similar results obtained in [19], Theorem III.2, and in [20], Lemma 3.1) which (up to extraction of subsequences) states that, as $\varepsilon\to 0$,

$$n^\varepsilon(t,x)\rightharpoonup n(t,x)=\int_{\mathbb{R}^3}f(t,x,\xi)\mathrm{d}\xi,\tag{3.3.6}$$

in $C([0,\tau];\mathcal{M}^+(\mathbb{R}^3_x)-w*)$. We therefore conclude $I^\varepsilon \to 0$, as $\varepsilon \to 0$, which consequently implies (3.3.4). In summary we have shown that the Wigner transformed evolution equation (3.3.3) converges weakly to

$$\int_0^\infty \iint_{\mathbb{R}^6} \Big(-\partial_t\sigma(t)\phi(x,\xi) - \frac{\xi}{\sqrt{|\xi|^2+1}} \cdot \nabla_x\phi(x,\xi)\sigma(t)\Big) f(t,x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}t$$
$$+ \int_0^\infty \iint_{\mathbb{R}^6} \sigma(t)\nabla_x V \cdot \nabla_\xi\phi(x,\xi) f(t,x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}t = \iint_{\mathbb{R}^6} \sigma(0)\phi(x,\xi) f_0(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi,$$

i.e. the relativistic Vlasov-Poisson system (in distributional sense). This finishes the proof. □

3.4 More general self-consistent potentials

It is straightforward to generalize the results discussed here for *Yukawa-type interactions*, i.e.

$$V^\varepsilon(t,x) = \kappa \frac{e^{-\lambda|x|}}{4\pi|x|} * n^\varepsilon(t,x), \quad \lambda > 0,$$

which are used in, e.g. [11]. Indeed it is possible to prove our main result for an even more general class of self-consistent interaction potentials $V^\varepsilon = G * n^\varepsilon$, if the kernel $G = G(x)$ satisfies the following regularity conditions:

$$\begin{aligned} &G^- \in L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \\ &\nabla G \in L^{10/7}(\mathbb{R}^3) + L^p(\mathbb{R}^3) \qquad \text{with} \quad \frac{10}{7} < \mathrm{p} < \infty \end{aligned} \tag{3.4.1}$$

where G^- is the negative part of $G = G^+ - G^-$. We write

$$\mathcal{E}^\varepsilon_{\text{pot}}(t) = \frac{1}{2}\operatorname{tr}((G^+ * n^\varepsilon)\rho^\varepsilon(t)) - \frac{1}{2}\operatorname{tr}((G^- * n^\varepsilon)\rho^\varepsilon(t)).$$

As we will explain in the sequel, the former assumption is required for the uniform a-priori bound of the kinetic energy (obviously, that is why the positive part G^+ does not require additional assumption) and the latter one is needed to carry the classical limit in the nonlinear term. If $G^- \in L^\infty(\mathbb{R}^3)$ then

$$\operatorname{tr}((G^- * n^\varepsilon)\rho^\varepsilon(t)) \le C \operatorname{tr}\rho^\varepsilon_0$$

and then the boundedness of the kinetic energy follows from the energy conservation immediately on each compact time interval $[0,\tau]$. But if $G^- \notin L^\infty(\mathbb{R}^3)$, we need to find a uniform bound of the negative part of the potential energy in terms of the kinetic energy considering the similar arguments discussed in the proof of Lemma 3.2.4. Recalling the Sobolev inequality

$$\iint_{\mathbb{R}^6} G^-(x-y)n^\varepsilon(t,x)n^\varepsilon(t,y)\mathrm{d}x\mathrm{d}y \le C_s \left\|G^-\right\|_{L^r} \|n^\varepsilon(t)\|^2_{L^q},$$

$$\text{with} \qquad \frac{2}{q}+\frac{1}{r}=2, \qquad 1\le q,r\le\infty.$$

Together with the interpolation estimates obtained in Lemma 3.2.1 desired bound is obtained with limit values $(r,q)=(5/2,5/4)$.

Now we should recover the time equicontinuity (for the compactness argument) only for the nonlinear term, that is

$$|\langle \Theta^\varepsilon[V^\varepsilon]f^\varepsilon,\phi\rangle| \le \|f^\varepsilon(t)\|_{L^2} \|\nabla_x V^\varepsilon(t)\|_{L^2} \| \sup_{y\in\mathbb{R}^3} |\hat{\phi}(y,\eta)||\eta| \,\|_{L^2} < \infty,$$

which holds true under the assumptions (3.4.1) since

$$\|\nabla_x V^\varepsilon(t)\|_{L^2} = \|\nabla G * n^\varepsilon(t)\|_{L^2} \le C\|n^\varepsilon(t)\|_{L^{5/4}}.$$

It remains to carry the limit to identify the cluster point. In the present situation we cannot use the regularizing property of the Poisson equation since we don't have it anymore. Instead we follow what is done in [19, 1]. Using the same notation after splitting the nonlinear term,

$$J^\varepsilon = \iint_\Omega |\nabla G * n(t,x+\varepsilon s\eta) - \nabla G * n(t,x)|^2 \mathrm{d}x\,\mathrm{d}\eta \longrightarrow 0$$

can be shown as above in the Section 3.3. So we need to show now that

$$I^\varepsilon = \iint_\Omega |\nabla G * n^\varepsilon(t,x+\varepsilon s\eta) - \nabla G * n(t,x+\varepsilon s\eta)|^2 \mathrm{d}x\,\mathrm{d}\eta \longrightarrow 0.$$

Since $z := x+\varepsilon s\eta \in \mathcal{O}$ (a compact of $\mathbb{R}^3$) it suffices if we show that $\nabla G * n^\varepsilon \to \nabla G * n$ in $C([0,\tau]; L^2_{\mathrm{loc}}(\mathbb{R}^3))^3$. By (3.4.1) we have $\nabla G = G_1 + G_2 \in L^{10/7}(\mathbb{R}^3)^3 + L^p(\mathbb{R}^3)^3$. Then let $g_n \in C_c(\mathbb{R}^3)^3$ be a vector sequence such that $g_n \to G_1$ in $L^{10/7}(\mathbb{R}^3)^3$ for $n\to\infty$ and with Ω_x a compact subset of $\mathbb{R}^3_x$. For $j=1,2,3$ we consider

$$\begin{aligned}\left\|G_1^j * n^\varepsilon(t) - G_1^j * n(t)\right\|_{L^2(\Omega_x)} \le& \left\|g_n^j * (n^\varepsilon - n)(t)\right\|_{L^2(\Omega_x)} \\ &+ \left\|(G_1^j - g_n^j) * (n^\varepsilon - n)(t)\right\|_{L^2(\Omega_x)} \\ :=& M^\varepsilon + N^\varepsilon.\end{aligned}$$

When $\varepsilon\to 0$ we have $n^\varepsilon(t,x) \rightharpoonup n(t,x)$ in $C([0,\tau];\mathcal{M}^+(\mathbb{R}^3_x)-w*)$ as in (3.3.6). This implies

$$M^\varepsilon \le |\Omega_x| \sup_{(t,x)\in[0,\tau]\times\Omega_x} |g_n^j * (n^\varepsilon - n)(t,x)| \longrightarrow 0.$$

Now noting that, up to subsequences, $n^\varepsilon \rightharpoonup n$ in $L^\infty([0,\tau]; L^{5/4}(\mathbb{R}^3)) - w*$, we have (by Young inequality)

$$
\begin{aligned}
N^\varepsilon &\leq \|G_1^j - g_n^j\|_{L^{10/7}(\mathbb{R}^3)} \|n^\varepsilon - n\|_{L^\infty([0,\tau];L^{5/4}(\mathbb{R}^3))} \\
&\leq C_\tau \|G_1^j - g_n^j\|_{L^{10/7}(\mathbb{R}^3)}
\end{aligned}
$$

where the last term is arbitrarily small for $n \to +\infty$ and independent of time. Thus we have proven that $G_1 * n^\varepsilon \quad \to \quad G_1 * n$ in $C([0,\tau]; L^2(\Omega_x))^3$. For the term $G_2 * n^\varepsilon$, one proceeds in a similar fashion what is done above to end up with the desired convergence for $\nabla G * n^\varepsilon$.

Remark 3.4.1. Finally, we remark that one can also treat the case of *semi-relativistic Hartree-Fock systems*, cf. [6], by combining straightforwardly the results present here with those given in [8] for non-relativistic Hartree-Fock systems. To this end, one should note that the so-called *exchange-term* vanishes as $\varepsilon \to 0$. Hence, one again recovers the relativistic Vlasov-Poisson system (3.1.9) in the limit.

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Part II

Thermal effects in gravitational Hartree systems

Chapter 4

Stable ground states of gravitational Hartree systems with temperature *

4.1 Introduction

4.1.1 Physical motivation and relations to other works

In this chapter we shall investigate the *gravitational Hartree system with temperature*. This model can be seen as a mean-field description for a system of self-gravitating quantum particles in non-relativistic regime. Applications arise mainly in astrophysics, for example in the description of so-called *Boson stars*. In particular, we shall be interested in *thermal effects*, arising for quantum systems at non-zero temperatures.

To this end, 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 $L^2(\mathbb{R}^3;\mathbb{C})$. The (kernel of the) integral operator ρ can be decomposed as

$$\rho = \sum_{j\in\mathbb{N}} \lambda_j |\psi_j\rangle\langle\psi_j| \tag{4.1.1}$$

where the non-negative eigenvalues $\lambda_j \in \ell^1$, $\lambda_j \geq 0$, describe the *occupation probabilities* within the set of eigenfunction $(\psi_j)_{j\in\mathbb{N}}$, forming a complete orthonormal basis of $L^2(\mathbb{R}^3)$, cf. [30]. By evaluating the kernel $\rho(x,y)$ on its diagonal, we obtain the corresponding particle density i.e.

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

*This chapter is a joint work with Jean Dolbeault and Christof Sparber.

In the following we shall assume that

$$\int_{\mathbb{R}^3} n_\rho(x)\,\mathrm{d}x = M, \tag{4.1.2}$$

for a given total mass $M > 0$. In the case of purely gravitational interactions, the *Hartree energy* of the system is 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* $V_\rho = n_\rho * \frac{1}{|\cdot|}$. Using the decomposition (4.1.1) the Hartree energy can be written as

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

In the following we shall consider an associated *free energy functional* given by

$$\mathcal{F}_T[\rho] := \mathcal{E}_H[\rho] - T\mathcal{S}[\rho], \tag{4.1.3}$$

with $T \geq 0$ denoting the temperature and $\mathcal{S}[\rho]$ the *entropy functional*

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

Here $\beta(s) \in \mathbb{R}_+$ is an *entropy generating function*, assumed to be convex (plus some additional properties to be prescribed later on, cf. Section 1.2).

The purpose of the present work is to investigate the existence and qualitative properties of *minimizers* for $\mathcal{F}_T[\rho]$ with temperature $T \geq 0$. These minimizers, usually referred to as *ground states*, can be interpreted as stationary states for the corresponding time-dependent system

$$i\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \left[H_{\rho(t)}, \rho(t)\right], \quad \rho(0) = \rho_{\mathrm{in}}, \tag{4.1.4}$$

where $[\cdot,\cdot]$ denotes the usual commutator and H_ρ the mean-field *Hamiltonian operator* i.e.

$$H_\rho := -\Delta - n_\rho * \frac{1}{|\cdot|}\,. \tag{4.1.5}$$

Using again the decomposition (4.1.1) for $\rho_{\mathrm{in}} \in \mathfrak{S}_1$, this can equivalently be rewritten as a system of countable many Schrödinger equation, coupled via the mean field potential V_ρ, i.e.

$$\begin{cases} i\partial_t\psi_j + \Delta\psi_j + V(t,x)\psi_j = 0, \quad j\in\mathbb{N}, \\ -\Delta V = 4\pi\sum_{j\in\mathbb{N}} \lambda_j|\psi_j(t,x)|^2. \end{cases} \tag{4.1.6}$$

This system is generalization of the gravitational Hartree equation (also known as *Schrödinger-Newton model* [6]) to the case of mixed states.

Establishing the existence of stationary solutions to nonlinear Schrödinger models such as (4.1.6) by means of a variational method, is a classical approach in mathematical physics, cf. [15]. A particular advantage of it, is that very often one can directly infer from it *orbital stability* of the stationary state the dynamics of (4.1.4), or, equivalently (4.1.6). In the case of *repulsive* self-consistent interactions, describing e.g. electrons, such an approach has been successfully carried out in [7, 8, 9, 24]. In addition, existence of stationary solutions for the repulsive case has been obtained in e.g. [23, 25, 26, 27], using convexity properties of the corresponding energy functional.

In sharp contrast to the repulsive case, the considered 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 $T = 0$, the free energy $\mathcal{F}_T[\rho]$ reduces to the classical gravitational Hartree energy. For this model, existence and uniqueness of the corresponding (zero temperature) ground states has been studied in [14] by using radially symmetric decreasing rearrangements. More recently in [6] the zero temperature problem, but in lower dimensions, has been studied by employing shooting methods. More interestingly in [17, 19] relying on the so-called *concentration-compactness method* introduced by Lions [18] has been employed to prove existence of minimizers of the Hartree energy. In particular, it is known that minima of the Hartree energy are achieved by *pure states*, i.e. rank one density matrices $\rho_0 = M|\psi_0\rangle\langle\psi_0|$. We further note that the concentration compactness method has recently been adapted to the setting of density matrix operators in [13], where the authors study a *semi-relativistic* model of Hartree-Fock type.

In view of these references, the goals of this chapter can be summarized as follows: First, we want to study the existence of minimizers for $\mathcal{F}_T[\rho]$, and thus extending the results of [14, 17, 19, 6] to the case of non-zero temperature. It turns out that in general we have to expect a *threshold in temperature*, as a consequence of the competition between the Hartree energy and the entropy term. In other words, we find that minimizers of $\mathcal{F}_T[\rho]$ in general only exist below a certain *maximal temperature* $T^* > 0$, depending on the specific form of the entropy generating function $\beta(s)$. To this end, one should note that, by using the scaling properties of the system, the notion of a maximal temperature (for a given mass $M > 0$) can then be rephrased into a corresponding threshold for the mass at a given (fixed) temperature T. The latter however, has to be clearly distinguished from the well-known *Chandrasekhar mass* threshold appearing in semi-relativistic models, such as [16, 11, 13]. Moreover, depending on the choice of β, it can be that $T^* = +\infty$, i.e. situations in which the temperature can be taken arbitrarily large for the minimizers of $\mathcal{F}_T[\rho]$ to still exist. Once the existence of minimizers has been established, a second goal of our work will be the study of qualitative properties of these ground states with respect to the temperature $T \in [0, T^*)$. In particular, we shall find 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.

We finally want to remark that there is a well-known analogue of our approach within the classical kinetic theory of self-gravitating systems. In this context, a variational approach based on so-called *Casimir functionals*, cf. [4], is employed to prove existence and stability of stationary states for (relativistic and non-relativistic) Vlasov-Poisson models, cf. [28, 29, 31, 32, 33] for more details. These functionals can be regarded as the classical counterpart of $\mathcal{F}_T[\rho]$, and we also refer to [24] for a closely related application in quantum mechanical application.

4.1.2 Mathematical setting and main result

In order to have a well-defined mathematical set-up, we first introduce the following Banach space of operators

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

equipped with the norm

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

The space $\mathfrak{H}$ can be interpreted as the space of density matrix operators with finite energy. Note that, by using the decomposition (4.1.1), we obtain from $\rho \in \mathfrak{H}$ that $\psi_j \in H^1(\mathbb{R}^3)$, for all $j \in \mathbb{N}$. By taking into account the mass constraint (4.1.2) we arise at the physical state space under consideration, i.e.

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

For $\rho \in \mathfrak{H}_M$, we denote the infimum of the free energy functional $\mathcal{F}_T[\rho]$ defined in (4.1.3) by

$$i_{M,T} = \inf_{\rho \in \mathfrak{H}_M} \mathcal{F}_T[\rho] \,. \tag{4.1.7}$$

As we shall see in the next section, $i_{M,T} < 0$, if it exists. The latter however, can only be guaranteed below a certain maximal temperature $T^* = T^*(M)$, i.e.

$$T^*(M) := \sup\{T > 0 \ : \ i_{M,T} < 0\}, \tag{4.1.8}$$

to be studied in more detail in Proposition 4.2.3 below. In particular, T^* will depend on the choice of the entropy generating function β, for which we assume:

(β1) β is strictly convex and of class C^1 on its domain: $\beta^{-1}([0,\infty))$.

(β2) β is nonnegative with $\beta(0) = \beta'(0) = 0$.

Remark 4.1.1. A typical example for the function β reads

$$\beta(s) = s^p, \quad 1 < p < 3. \tag{4.1.9}$$

Such power law distributions are of common use in the classical kinetic theory of self-gravitating systems, since they explain the existence and stability of so-called *polytropic galaxies* and in addition give rise to stationary states with compact support, cf. [10, 28, 29, 31, 32, 33]. One should also note that the common choice $\beta(s) = s \ln s$ yields a free energy functional which is *unbounded* from below [21].

We are now in the position to state our main mathematical result.

Theorem 3. *Let $M > 0$ and $T^* = T^*(M) > 0$ be the, possibly infinite, maximal temperature defined in* (4.1.8). *Then it holds:*

(i) For all $T < T^*$, there exists an operator ρ in $\mathfrak{H}_M$ such that $\mathcal{F}_T[\rho] = i_{M,T}$.

(ii) The set of all minimizers $\mathfrak{M}_M \subset \mathfrak{H}_M$ is orbitally stable under the dynamics of (4.1.4)*, see Corollary 4.5.1 for more details.*

(iii) Minimizer $\rho \in \mathfrak{M}_M$ are pure states, i.e. density matrix operators of rank one, if and only if $T \in [0, T_c]$, where $T_c > 0$ is a well-defined critical temperature.

The proof of this theorem will be a consequence of several results established in the upcoming sections. To this end, we shall rely on the concentration compactness method (in density matrix framework) similarly to [13]. In comparison to the latter, several adaptations have to be made in order to deal with the case of non-zero temperatures.

Remark 4.1.2. So far, we do not know about uniqueness of minimizers $\rho \in \mathfrak{M}_M$, except for the case of zero temperature $T = 0$, where uniqueness has been proved in [14]. See also [12] for an analogous result in the semi-relativistic case.

The chapter is organized as follows: In Section 4.2 we collect several basic properties of the free energy. In particular we shall exhibit the existence of a maximal temperature T^*. In Section 4.3 we state two important a-priori estimates for the minimizers which will be used in the existence proof given in Section 4.4. After establishing the existence of minimizers we shall study their properties in more detail in Section 4.5 including the question of whether minimizers are pure or mixed states.

4.2 Basic properties of the free energy

4.2.1 Boundedness from below and splitting property

As a preliminary step for the existence of minimizers we have to guarantee that the functional $\mathcal{F}_T[\rho]$ is well defined and $i_{M,T} > -\infty$.

Lemma 4.2.1. *The free energy $\mathcal{F}_T$ introduced in* (4.1.3) *is well-defined and bounded from below for all $\rho \in \mathfrak{H}_M$. If $\mathcal{F}_T[\rho]$ is finite, then $\sqrt{n_\rho}$ is bounded in $H^1(\mathbb{R}^3)$.*

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

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

by the Hardy-Littlewood-Sobolev inequality. Next, by Sobolev's embedding, we know that $\|n_\rho\|_{L^3}$ is controlled by $\left\|\nabla \sqrt{n_\rho}\right\|_{L^2}^2$ which, using the decomposition (4.1.1), is bounded by $\operatorname{tr}(-\Delta\rho)$. Hence we can conclude that

$$\mathcal{E}_{\text{pot}}[\rho] \leq C \, \|n_\rho\|_{L^1}^{3/2} \operatorname{tr}(-\Delta\rho)^{1/2} \tag{4.2.1}$$

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

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

For the entropy term $\mathcal{S}[\rho] = -\operatorname{tr}\beta(\rho)$ we note that, since β is convex and $\beta(0) = 0$, it holds $0 \leq \beta(\rho) \leq \beta(1)\rho$ for all $\rho \in \mathfrak{H}$ and $\beta(\rho) \in \mathfrak{S}_1$, provided $\rho \in \mathfrak{S}_1$. Hence, all quantities involved in the definition of $\mathcal{F}_T$ are well-defined and bounded on $\mathfrak{H}_M$. $\square$

Throughout this work, we shall frequently use the following smooth *cut-off functions*: Let $0 \leq \chi \leq 1$ be a fixed smooth function on $\mathbb{R}^3$, such that $\chi \equiv 1$ for $|x| < 1$ and $\chi \equiv 0$ for $|x| \geq 2$. For any $R > 0$, the we consequently define cut-off functions χ_R and ξ_R via

$$\chi_R(x) = \chi(x/R) \quad \xi_R(x) = \sqrt{1 - \chi(x/R)^2}. \tag{4.2.2}$$

The motivation for introducing these cut-off functions, is that for any function $u \in H^1(\mathbb{R}^3)$, we have

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

and the IMS truncation identity,

$$\int_{\mathbb{R}^3} |\nabla(\chi_R u)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^3} |\nabla(\xi_R u)|^2 \,\mathrm{d}x = \int_{\mathbb{R}^3} |\nabla u|^2 \,\mathrm{d}x - \int_{\mathbb{R}^3} |u|^2 \underbrace{\nabla \cdot (\nabla \chi_R + \nabla \xi_R)}_{=O(R^{-2}) \text{ as } R\to\infty} \,\mathrm{d}x. \tag{4.2.3}$$

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

Lemma 4.2.2. *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:*

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

As a consequence, we obtain

$$\mathcal{F}_T[\rho_R^{(1)}] + \mathcal{F}_T[\rho_R^{(2)}] \leq \mathcal{F}_T[\rho] + O(R^{-2}), \quad \text{as } R \to +\infty.$$

Proof. The assertion for the Hartree energy $\mathcal{E}_H[\rho]$ is a straightforward consequence of (4.2.3). For the entropy term, we can use the celebrated *Brown-Kosaki inequality*, in the same way as in [7, Lemma 3.4] to obtain

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

Since, by definition, $\mathcal{F}_T[\rho] = \mathcal{E}_H[\rho] + T \operatorname{tr} \beta(\rho)$, with $T \geq 0$, the lemma is proved. $\square$

4.2.2 Sub-additivity and maximal temperature

In order to proceed further, we need to study the properties of $i_{M,T}$ with respect to its parameters M and T. In particular, we shall establish the occurrence of a maximal temperature $T^*(M)$ as defined in (4.1.8). To this end, we have to take into account the translation invariance of the model and denote by, for a given $y \in \mathbb{R}^3$, the (unitary) translation operator $\tau_y : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ by

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

Proposition 4.2.3. *Let $i_{M,T}$ be given by* (4.1.7)*. Then, the following properties hold:*

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

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

(ii) The function $i_{M,T}$ is a decreasing function of M and an increasing function of T and, for any $T < T^*$, we have $i_{M,T} < 0$.

(iii) For any $M > 0$, $T^*(M) > 0$ is positive, maybe even 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, we know that $T^*(M) > 0$, 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. To this end, consider two states $\rho \in \mathfrak{H}_{M-m}$ and $\sigma \in \mathfrak{H}_m$, such that $\mathcal{F}_T[\rho] \leq i_{M-m,T} + \varepsilon$ and $\mathcal{F}_T[\sigma] \leq i_{m,T} + \varepsilon$. By density of finite rank operators in $\mathfrak{H}$ and of C_0^∞ in L^2, we can assume that

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

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

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

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

Next, consider the minimizer ρ_0 of $\mathcal{E}_H$, subject to $\operatorname{tr}\rho = M$. (It is given by the an appropriately re-scaling of the pure state obtained in [14].) Given $\lambda \in \mathbb{R}_+$, let $(U_\lambda f)(x) := \lambda^{3/2} f(\lambda x)$, and observe that $\rho_\lambda = U_\lambda \rho_0 {U_\lambda}^* \in \mathfrak{H}_M$. Computing $\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathcal{E}_H[\rho_\lambda] = 0$, we infer that $\lambda = \mathcal{E}_{\mathrm{pot}}/(2\mathcal{E}_{\mathrm{kin}})$, and thus

$$i_{M,0} \equiv \mathcal{E}_H[\rho_0] = -\frac{1}{4} \frac{\mathcal{E}_{\mathrm{pot}}^2[\rho_0]}{\operatorname{tr}(-\Delta\rho_0)} \, .$$

As a consequence, we have $i_{M,0} = M^3 \; i_{1,0}$ since for temperature $T = 0$ the minimal energy is homogeneous. Moreover, we have

$$\mathcal{F}_T[\rho] = i_{M,0} + T\beta(M) = \beta(M)\left(T - \frac{M^3}{\beta(M)}|i_{1,0}|\right) \geq i_{M,T} \, , \tag{4.2.4}$$

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

Next, $M \mapsto i_{M,T}$ is a decreasing function of M as a consequence of the sub-additivity property and $T \mapsto i_{M,T}$ is an increasing function of T because, by assumption, β takes positive values on $(0, \infty)$. As a consequence, $T^*(M)$ is an increasing function of M, such that

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

By the sub-additivity inequality and (4.2.4), we obtain

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

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 $n \to \infty$. 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 (4.2.4), we infer

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

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 $T < T^*(M)$. ☐

Remark 4.2.4. If equality holds in Lemma 4.2.3 part *(iii)* for some M and m, then there exists a minimizing sequence for $i_{M,T}$ that is not relatively compact in $\mathfrak{H}$ up to translations. This can be seen by taking two minimizing sequences ρ_n (for $i_{m,T}$) and ρ'_n (for $i_{M-m,T}$) of finite rank operators with decomposition in smooth functions, compactly supported in centered balls of radius R_n, as in the proof of sub-additivity property. Then we translate one of them and obtain a minimizing sequence $\rho_n + \tau_{3R_n e} \rho'_n \tau^*_{3R_n e}$ for $i_{M,T}$ which fails to be relatively compact in $\mathfrak{H}_M$, even up to translations, as n tends to infinity. In the language of the concentration-compactness method, *dichotomy* occurs.

Remark 4.2.5. By choosing β as in (4.1.9) numerical computations for T^* are currently being carried out for different values of p, see the upcoming work [1]. The numerical codes are thereby adapted from methods in quantum chemistry.

4.3 A-priori estimates for minimizers

In this section we shall establish two important a-priori estimates for minimizers $\rho \in \mathfrak{H}_M$ of $\mathcal{F}_T[\rho]$, assuming that they exist.

4.3.1 A decay property of the spatial density

As a first step we shall establish a result which is the analog of [13, Lemma 5.2].

Proposition 4.3.1. *Let $\rho \in \mathfrak{H}_M$ be a minimizer for $\mathcal{F}_T[\rho]$. Then there exists a constant $C > 0$ such that*

$$\int_{|x|>R} n_\rho(x)\,\mathrm{d}x \leq \frac{C}{R^2}, \tag{4.3.1}$$

for all $R > 0$ sufficiently large.

Proof. We follow the proof given in [13]: Let $\mu < 0$ be the Lagrange multiplier obtained in Proposition 4.5.3 and consider on $\mathfrak{H}$ the linear functional

$$\gamma \mapsto \mathrm{tr}\left[(H_\rho - \mu + T\,\beta'(\rho))\,\gamma\right] =: L_\mu[\gamma]\ .$$

We claim that the minimizer $\rho \in \mathfrak{H}_M$ for $i_{M,T}$ also minimizes the linear functional $L_\mu[\gamma]$ on $\mathfrak{H}$. To see this, consider the following minimization problem

$$l_M = \inf_{\gamma\in\mathfrak{H}_M} L[\gamma], \quad L[\gamma] = \mathrm{tr}\,(H_\rho + T\,\beta'(\rho))\,\gamma\ .$$

It will become clear from the results given in Section 4.5.2 that $L[\rho] = \inf_{\gamma\in\mathfrak{H}_M} L[\gamma]$. Next, we observe that the map $M \mapsto l_M$, i.e. $\mathrm{tr}\,\gamma \mapsto l_{\mathrm{tr}\,\gamma}$ is convex (since L is linear) which yields

$$l_m \geq l_M + \mu(m - M), \qquad \text{for all} \quad m \geq 0\ , \tag{4.3.2}$$

whenever $\mu \in [l_M^-, l_M^+]$, where l_M^- and l_M^+ denote the left and right derivatives of l_M, respectively. Since $M \mapsto l_M$ is convex and nonincreasing (see Lemma 4.2.3) $\mu < 0$ holds. Then we conclude from (4.3.2) the following estimate

$$\inf_{\gamma\in\mathfrak{H}_m} \mathrm{tr}[(H_\rho + T\beta'(\rho) - \mu)\gamma] \geq \inf_{\gamma\in\mathfrak{H}_M} \mathrm{tr}[(H_\rho + T\beta'(\rho) - \mu)\gamma] = L[\rho] - \mu\,\mathrm{tr}\,\rho = L_\mu[\rho].$$

Thus we obtain $\inf_{\gamma\in\mathfrak{H}} L_\mu[\gamma] = L_\mu[\rho]$. Hence ρ minimizes $L_\mu[\gamma]$ on $\mathfrak{H}$.

Next we introduce $\rho_R = \chi_R\rho\chi_R$ where we recall (4.2.2) for the definition of cutoff functions. We claim that

$$L_\mu[\rho_R] \leq L_\mu[\rho] - \mathrm{tr}(-\Delta\xi_R\rho\xi_R) + (\mu + o(1)) \int \xi_R^2(x) n_\rho(x)\,\mathrm{d}x + \frac{C}{R^2} \tag{4.3.3}$$

holds as $R > 0$ sufficiently large. On the other hand we have that $L_\mu[\rho_R] \geq L_\mu[\rho]$, since ρ is the minimizer for $L_\mu[\gamma]$. Thus, having in mind that $\mu < 0$), we can deduce the following inequality (provided (4.3.3) holds true)

$$\mathrm{tr}((-\Delta)\xi_R\rho\xi_R) + \int \xi_R^2(x) n_\rho(x)\,\mathrm{d}x \leq \frac{C}{R^2} \quad \text{for } R \geq R_0.$$

for some sufficiently large constant $R_0 > 0$, which implies the desired estimate (4.3.1).

It remains to prove (4.3.3): For the kinetic energy we employ IMS localization formula (4.2.3) and deduce

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

And for the entropy term we use Brown-Kosaki's inequality to infer (see e.g. [7])

$$\mathrm{tr}\,\beta(\rho) \geq \mathrm{tr}\,\beta(\rho_R) + \mathrm{tr}\,\beta(\xi_R\rho\xi_R)\,.$$

Now, we rewrite the potential energy as follows:

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

To treat the second integral we use the fact that $|x-y| \geq \frac{3R}{4}$, whereas for the third term on the r.h.s. we use

$$\begin{aligned}\left\|\xi_{R/4}^2 n * 1/|x|\right\|_{L^\infty} &\leq C\left\|\xi_{R/4}^2 n\right\|_{L^3}^{1/3}\left\|\xi_R^2 n\right\|_{L^{6/5}}^{2/3} \leq C(\mathrm{tr}(-\Delta\xi_R\rho\xi_R))^{1/2}\\ &\leq C(\mathrm{tr}([-\Delta,\xi_R^2]\rho))^{1/2} + (\mathrm{tr}(\xi_R(-\Delta\rho)\xi_R))^{1/2} \leq \frac{C}{R} + o(1)\,.\end{aligned}$$

In summary this yields

$$\mathcal{E}_{\mathrm{pot}}[\rho] \leq \mathrm{tr}\,V_\rho\rho_R + \left(\frac{C}{R} + o(1)\right)\int \xi_R^2(x)n_\rho(x)\mathrm{d}x.$$

Combining this with the already established estimates for the kinetic energy and the entropy finishes the proof of (4.3.3). $\square$

4.3.2 Binding inequalities

As a consequence of Proposition 4.3.1, we can prove the following strict subadditivity property of $i_{M,T}$, usually called *binding inequality*, see e.g. [13].

Corollary 4.3.2. *Let $M^{(1)} > 0$ and $M^{(2)} > 0$. If there are minimizers for $i_{M^{(1)},T}$ and $i_{M^{(2)},T}$, then*

$$i_{M^{(1)}+M^{(2)},T} < i_{M^{(1)},T} + i_{M^{(2)},T}\,. \tag{4.3.4}$$

Proof. We consider two minimizers $\rho^{(1)}$ and $\rho^{(2)}$ for $i_{M^{(1)},T}$ and $i_{M^{(2)},T}$, respectively. First, we claim that

$$\mathcal{F}_T[\chi_R\,\rho^{(\ell)}\,\chi_R] \geq i_{M^\ell,T} + \frac{C}{R^2}, \quad \text{and} \quad \ell = 1,2\,, \tag{4.3.5}$$

for any $R > 0$ sufficiently large, where χ_R is the cutoff function given in (4.2.2), as well as ξ_R for future reference.

We shall only give the proof for $\ell = 1$, since the case $\ell = 2$ is similar. As before, for the kinetic energy we employ the localization formula to obtain

$$\mathrm{tr}(-\Delta\rho^{(1)}) \geq \mathrm{tr}(-\Delta\chi_R\rho^{(1)}\chi_R) - \frac{C}{R^2}\,.$$

and by the Brown-Kosaki inequality, we also have that

$$\mathrm{tr}\,\beta(\rho^{(1)}) \geq \mathrm{tr}\,\beta(\chi_R\rho^{(1)}\chi_R)\,.$$

It remains to treat the potential energies. Using the fact that $\chi_R^2 + \xi_R^2 = 1$ and the symmetry w.r.t. x and y, we can estimate

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

for $R > 0$ large enough. Since

$$\left\| n_{\rho^{(1)}} * \frac{1}{|\cdot|} \right\|_{L^\infty(\mathbb{R}^3)} \leq C(\mathrm{tr}(-\Delta\rho^{(1)}))^{1/2},$$

and having in mind the decay estimate for the minimizer $\rho^{(1)}$ as given Lemma 4.3.1, we obtain

$$\left|\mathcal{E}_{\mathrm{pot}}[\rho^{(1)}] - \mathcal{E}_{\mathrm{pot}}[\chi_R\rho^{(1)}\chi_R]\right| \leq C\int_{|x|\geq R} n_{\rho^{(1)}}(x)\,\mathrm{d}x \leq \frac{C}{R^2}.$$

This concludes the proof of (4.3.5).

Next, we prove (4.3.4). To this end (as in [13]) we start with a test state

$$\rho_R := U\chi_R\rho^{(1)}\chi_R U^* + \tau_{5R\nu}V\chi_R\rho^{(2)}\chi_R V^*\tau_{5R\nu}^*$$

for some unit vector $\nu \in \mathbb{S}^2$ and some rotations $U, V \in SO(3)$ which will be useful in the use of Newton's theorem. As χ_R and $\tau_{5Re}\chi_R$ have disjoint supports $\rho_R \in \mathfrak{H}$. Moreover, we have

$$\mathrm{tr}\,\rho_R = \mathrm{tr}\,\chi_R\rho^{(1)}\chi_R + \mathrm{tr}\,\xi_R\rho^{(1)}\xi_R \leq M^{(1)} + M^{(2)}\,.$$

And we note that the free energy is rotation and translation invariant, i.e. $\mathcal{F}_T[\rho] = \mathcal{F}_T[\tau_y U \rho U^* \tau_y^*]$ for all $y \in \mathbb{R}^3$ and $U \in SO(3)$. Newton's theorem says, for radial functions,

$$\int \frac{f(x)}{|x-y|} \, \mathrm{d}x \leq \frac{\int f \, \mathrm{d}x}{|x|} \, .$$

Having in mind that the map $M \mapsto i_M$ is decreasing, one can obtain the following estimate, cf. [13]:

$$\begin{aligned} i_{M^{(1)}+M^{(2)},T} &\leq \iint_{SO(3)\times SO(3)} \mathcal{F}_T[\rho_R] \, \mathrm{d}U \mathrm{d}V \\ &\leq \mathcal{F}_T[\chi_R \rho^{(1)} \chi_R] + \mathcal{F}_T[\chi_R \rho^{(2)} \chi_R] - \frac{M^{(1)} M^{(2)}}{R} \\ &\leq i_{M^{(1)},T} + i_{M^{(2)},T} + \frac{C}{R^2} - \frac{M^{(1)} M^{(2)}}{R} \, . \end{aligned}$$

which yields the desired result for R sufficiently large. ☐

4.4 Existence of minimizers below T^*

In this section the basic existence result for ground states with temperature will be given. To this end, we shall need the following important property for minimizing sequences $(\rho_\ell)_{\ell\in\mathbb{N}} \in \mathfrak{H}_M$.

4.4.1 Conservation of mass implies compactness

As a final preliminary step, we shall recall the following convergence result for minimizing sequences to be used later on.

Lemma 4.4.1. *Let $(\rho_\ell)_{\ell\in\mathbb{N}} \in \mathfrak{H}_M$ be a minimizing sequence for $\mathcal{F}_T[\rho]$, such that, as $\ell \to \infty$: $\rho_\ell \rightharpoonup \rho$ weak$-*$ in $\mathfrak{H}$ and $n_{\rho_\ell} \to n_\rho$ almost everywhere. Then $\rho_\ell \to \rho$ strongly in $\mathfrak{H}$ if and only if $\operatorname{tr} \rho = M$.*

Proof. This result is classical, see e.g. [13, Corollary 4.1]. The proof relies on a characterization of the compactness due to Brezis and Lieb, see [2] and [15, Theorem 1.9], from which it follows that

$$\lim_{\ell\to\infty} \left(\int_{\mathbb{R}^3} n_{\rho_\ell} \, \mathrm{d}x - \int_{\mathbb{R}^3} |n_\rho - n_{\rho_\ell}| \, \mathrm{d}x \right) = \int_{\mathbb{R}^3} n_\rho \, \mathrm{d}x \, ,$$

and likewise

$$\lim_{\ell\to\infty} \Big(\operatorname{tr}(-\Delta\rho) - \operatorname{tr}\big(-\Delta(\rho - \rho_\ell) \big) \Big) = \operatorname{tr}(-\Delta\rho) \, .$$

By semi-continuity of $\mathcal{F}_T$ and compactness of the quadratic term in $\mathcal{E}_H$, we conclude that $\lim_{\ell\to\infty} \mathrm{tr}(-\Delta(\rho-\rho_\ell)) = 0$. $\square$

4.4.2 Existence of minimizers

Consider a minimizing sequence $(\rho_n)_{n\in\mathbb{N}}$ for $\mathcal{F}_T[\rho]$ 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, up to extraction of subsequences, $\tau_{a_n}^*\rho_n\tau_{a_n}$ strongly converges as $n\to\infty$. Clearly, the sub-additivity inequality for $\mathcal{F}_T[\rho]$ given in Lemma 4.2.3 (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 4.2.3, 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 4.3.2. To this end, the main issue will be to prove the convergence of two subsequences towards minimizers of mass smaller than M.

Proposition 4.4.2. *Let $M>0$ and consider $T^*=T^*(M)$ defined by* (4.1.8). *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 [13]. Compared to previous results (see for instance [20, 21, 22, 13]), the main difficulty arises in the splitting case, as we shall see below.

Step 1: Non-vanishing. We split

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

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 4.2.1, by Young's inequality we can estimate I_1 by

$$I_1 \le \|n_{\rho_n}\|^2_{L^{7/5}(\mathbb{R}^3)} \left\| \frac{1}{|\cdot|} \right\|_{L^{7/4}(B_{1/R})} \le \frac{C}{R^{5/7}}\ ,$$

and directly get bounds on I_2 and I_3 by computing

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

$$I_3 \le \frac{1}{R} \iint_{\mathbb{R}^6} n_{\rho_n}(x)\, n_{\rho_n}(y) \le \frac{M^{(2)}}{R}\ .$$

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

$$2\pi\, \mathcal{F}_T[\rho_n] \geq 2\pi\, i_{M,T} > -I_1 - I_2 - I_3$$

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

$$\sup_{y\in\mathbb{R}^3} \int_{a_n+B_R} n_{\rho_n}(x)\,\mathrm{d}x \geq \frac{1}{R\,M}\left(-2\pi\, i_{M,T} - \frac{M^{(2)}}{R} - \frac{C}{R^{5/7}}\right) > 0$$

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 4.4.1, or $M^{(1)} \in (0, M)$. Let us choose R_n such that $\int_{\mathbb{R}^3} n_{\rho_n^{(1)}}\,\mathrm{d}x = M^{(1)}$ where $\rho_n^{(1)} := \chi_{R_n}\,\rho_n\,\chi_{R_n}$. Let $\rho_n^{(2)} := \xi_{R_n}\,\rho_n\,\xi_{R_n}$. Since $\rho^{(1)}$ has a non-compact support, $\lim_{n\to\infty} R_n = \infty$. By Step 1, we know that $\rho_n^{(1)}$ strongly converges to $\rho^{(1)}$. By Identity (4.2.3) and Lemma 4.2.2, we find that

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

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 (Lemma 4.2.3, (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 Lemma 4.2.3, (ii), 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 Lemmata 4.3.2 and 4.2.3, (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. □

4.5 Ground state properties

Having established the existence of minimizers $\rho \in \mathfrak{H}_M$ of $\mathcal{F}_T[\rho]$, we shall now study their properties in more detail.

4.5.1 Orbital Stability

A direct consequence of our variational approach is the *orbital stability* of the set of minimizers $\mathfrak{M}_M \subset \mathfrak{H}_M$ under the dynamics of (4.1.4). To this end, we denote

$$\mathrm{dist}_{\mathfrak{M}_M}(\rho(t), \rho) = \inf_{\rho \in \mathfrak{M}_M} \|\rho(t) - \rho\| .$$

where $\rho(t)$ solved (4.1.4).

Corollary 4.5.1. *For given $M > 0$ let $T < T^*(M)$. Then for any $\varepsilon > 0$, there exists $\delta > 0$ such that, for all $\rho_{\rm in} \in \mathfrak{H}_M$ and $\rho \in \mathfrak{M}_M$ with $\mathrm{dist}_{\mathfrak{M}_M}(\rho_{\rm in}, \rho) \leq \delta$ it holds:*

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

where $\rho(t)$ is the solution of (4.1.4) *with the initial data $\rho_{\rm in}$.*

Remark 4.5.2. The same result is established in [24] for the case of repulsive Coulomb interactions.

Proof. As in [5] the result is a direct consequence of the conservation of the free energy along the flow and the compactness of all minimizing sequences. $\square$

4.5.2 Euler-Lagrange equations

Since $\mathcal{F}_T[\rho]$ is conserved along the Hartree dynamics, its minimizers $\rho \in \mathfrak{M}_M$ form stationary states of (4.1.4), i.e. they satisfy $[H_\rho, \rho] = 0$. In order to get more insight on their structure we can use the decomposition (4.1.1) and rewrite the stationary Hartree model in terms of countable many (nonlinear) eigenvalue problem

$$\begin{cases} \Delta\psi_j + V\psi_j + \mu_j\,\psi_j = 0, \quad j \in \mathbb{N}, \\ -\Delta V = 4\pi \displaystyle\sum_{j \in \mathbb{N}} \lambda_j |\psi_j|^2, \end{cases} \tag{4.5.1}$$

where $(\mu_j)_{k \in \mathbb{N}} \in \mathbb{R}_-$ denote the energy eigenvalues of the Hamiltonian H_ρ defined in (4.1.5). To this end, we have used the fact that one can diagonalize the eigenvalue matrix of $(\mu_{j,\ell})_{j,\ell \in \mathbb{N}}$ by a unitary transformation (i.e. a rotation). We further note that the system (4.5.1) has to be understood for $(\psi_j)_{j \in \mathbb{N}} \in H^1(\mathbb{R}^3)$, i.e. in the weak sense. As in [7, 24], we can characterize the sequence of occupation numbers $(\lambda_j)_{j \in \mathbb{N}}$ in terms of the eigenvalues $(\mu_j)_{k \in \mathbb{N}}$ and vice versa.

Proposition 4.5.3. *Let $M > 0$, $T < T^*(M)$ and consider a density matrix operator $\rho \in \mathfrak{H}_M$ which minimizes $\mathcal{F}_T[\rho]$. Then ρ satisfies the self-consistent equation*

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

where $\mu \leq 0$ denotes the Lagrange multiplier associated to the mass constraint. Explicitly, it is given by

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

The Lagrange multiplier μ is usually referred to as the *chemical potential.*

Proof. We will follow a classical approach to compute Euler-Lagrange equations of the free energy functional:

$$\mathcal{F}_T[\rho] = \operatorname{tr}\left(-\Delta\rho\right) - \frac{1}{2}\operatorname{tr}(V[\rho]\rho) + T\operatorname{tr}\beta(\rho)$$

under the constraint

$$\mathcal{G}[\rho] := \operatorname{tr}\rho \equiv M.$$

As a first step we introduce, for γ to be a trace class operator,

$$g(s,r) := \mathcal{G}(\rho + s\rho + r\gamma),$$

and then evaluate

$$\begin{aligned} \partial_s g(s,r) &= \operatorname{tr}\rho \\ \partial_r g(s,r) &= \operatorname{tr}\gamma, \end{aligned}$$

and observe that,

$$\partial_s g(0,0) \neq 0$$

and by the implicit function theorem the map $r \mapsto s(r)$ is C^1 such that $s(0) = 0$ and for all sufficiently small r we have

$$g(s(r), r) = M,$$

and this implies

$$\partial_r g(s(r), r) + \partial_s q(s(r), r)s'(r) = 0,$$

which leads to

$$s'(0) = -\frac{\operatorname{tr}\gamma}{\operatorname{tr}\rho}. \tag{4.5.2}$$

As a second step, we set

$$\begin{aligned} e(r) :=& \mathcal{F}_T[\rho + s(r)\rho + r\gamma] \\ =& \operatorname{tr}(-\Delta(\rho + s\rho + r\gamma)) - \frac{1}{2}\operatorname{tr}(V[\rho + s(r)\rho + r\gamma](\rho + s\rho + r\gamma)) \\ &\qquad + T\operatorname{tr}\beta(\rho + s\rho + r\gamma) \end{aligned}$$

and $e(r)$ attains its minimum at $r = 0$ which implies $e'(0) = 0$:

$$\begin{aligned} e'(0) =& \operatorname{tr}(-\Delta(s'(0)\rho + \gamma)) - \frac{1}{2}\operatorname{tr}(V[\rho](s'(0)\rho + \gamma)) \\ & - \frac{1}{2}\operatorname{tr}\left(\frac{\mathrm{d}}{\mathrm{d}r}V[\rho + s(r)\rho + r\gamma]\mid_{r=0}\rho\right) + T\operatorname{tr}(\beta'(\rho)(s'(0)\rho + \gamma)) \\ =& 0. \end{aligned} \tag{4.5.3}$$

Now we define $U := \frac{\mathrm{d}}{\mathrm{d}r}V[\rho + s(r)\rho + r\gamma]\mid_{r=0}$ then we have

$$\Delta U(x) = s'(0)\rho(x,x) + \Delta z.$$

where $\Delta z = w(x,x)$ which leads to $U = s'(0)V[\rho] + z$. Now we rewrite (4.5.3):

$$\begin{aligned} e'(0) =& s'(0)\operatorname{tr}(-\Delta\rho) + \operatorname{tr}(-\Delta\gamma) - s'(0)\operatorname{tr}(V[\rho](\rho)) \\ & - \operatorname{tr}(V[\rho]\gamma) + \operatorname{tr}(z\rho) + s'(0)T\operatorname{tr}(\beta'(\rho)\rho) + T\operatorname{tr}(\beta'(\rho)\gamma) \\ =& 0. \end{aligned}$$

Now we claim that $\operatorname{tr}(V[\rho]\gamma) = \operatorname{tr}(z\rho)$, and postpone the proof of this claim to the end in order to keep the coherence. Thus we arrange what we have above

$$0 = s'(0)\operatorname{tr}(H_\rho\rho + T\beta'(\rho)\rho) + \operatorname{tr}(H_\rho\gamma + T\beta'(\rho)\gamma), \qquad H_\rho = -\Delta - V[\rho].$$

Using (4.5.2) we obtain

$$0 = -\mu\operatorname{tr}\gamma + \operatorname{tr}(H_\rho\gamma + T\beta'(\rho)\gamma), \tag{4.5.4}$$

where

$$\mu = \frac{\operatorname{tr}(H_\rho\rho + T\beta'(\rho)\rho)}{\operatorname{tr}\rho}.$$

We point out that since β' is convex, then $\langle\beta'(\rho)\psi_k, \psi_k\rangle = \beta'(\lambda_k)$, where $\langle\cdot,\cdot\rangle$ denotes the inner product in $L^2(\mathbb{R}^3)$. This yields $\beta'(\rho)\psi_k = \beta'(\lambda_k)\psi_k$. Then we obtain from (4.5.4)

$$\sum_{k\in\mathbb{N}}\langle H_\rho\gamma\psi_k, \psi_k\rangle = \sum_{k\in\mathbb{N}}\left\langle(\mu - T\beta'(\lambda_k))\,\gamma\psi_k, \psi_k\right\rangle. \tag{4.5.5}$$

Now, we choose $\gamma = P_K$, which is the L^2-projection operator on the eigenstate ψ_K, i.e. for K fixed,

$$P_K\psi_k = \begin{cases} \psi_K & \text{if } k = K \\ 0 & \text{if } k \neq K \end{cases}.$$

This implies, for every K,

$$H_\rho\psi_K = (\mu - T\beta'(\lambda_K))\,\psi_K, \tag{4.5.6}$$

which proves that minimizers ρ of the free energy (4.1.3) are the steady states of the time-dependent system.

It remains to show that $\mu \leq 0$. To this end, we note that since the entropy term is convex, ρ is a minimizer not only for $\mathcal{F}_T[\rho]$ but also for the functional $\gamma \mapsto \operatorname{tr}((H_\rho + T\beta(\rho))\gamma)$ on $\mathfrak{H}_M$. Since the essential spectrum of H_ρ is $[0,\infty)$, μ cannot be positive.

Now we close the gap, namely the equality $\operatorname{tr}(V[\rho]w) = \operatorname{tr}(z\rho)$, where the act of the trace class operator w can be written as

$$wf = \sum_{k\in\mathbb{N}} \alpha_k \psi_k \langle f, \psi_k \rangle .$$

Now let us compute the trace keeping in mind that $w(x,x) = \Delta z$

$$\begin{aligned}
\operatorname{tr}(V[\rho]w) &= \sum_{k\in\mathbb{N}} \langle V[\rho]w\psi_k, \psi_k\rangle \\
&= \int_{\mathbb{R}} V[\rho] \sum_{k\in\mathbb{N}} \alpha_k |\psi_k|^2 \mathrm{d}x \\
&= \int_{\mathbb{R}} V[\rho]\Delta z \mathrm{d}x \\
&= \int_{\mathbb{R}} \Delta V[\rho] z \mathrm{d}x \\
&= \int_{\mathbb{R}} \rho(x,x) z \mathrm{d}x = \operatorname{tr}(z\rho).
\end{aligned}$$

This finishes the proof.

□

The stationary equation (4.5.6) means that the energy eigenvalues are written in terms of the occupation probabilities, i.e.

$$\mu_j = \mu - T\beta'(\lambda_j) \quad \text{provided } \mu_j \leq \mu. \tag{4.5.7}$$

From this, we obviously get that $\mu_j = \mu$ in the case of zero temperature $T = 0$.

4.5.3 Critical Temperature for mixed states

In this subsection, we shall deduce the existence a critical temperature $T_c \in (0, T^*)$, depending on the entropy function β, above which minimizers $\rho \in \mathfrak{M}_M$ become mixed states. To this end, we introduce the following notation: Let $\rho_0 = M|\psi_0\rangle\langle\psi_0|$ be the (appropriately scaled) minimizer for $T = 0$ obtained in [14]. Denote by

$$H_0 := -\Delta - |\psi_0|^2 * \frac{1}{|\cdot|}. \tag{4.5.8}$$

the corresponding Hamiltonian operator. From the results given in [14] it is clear that (the linear operator) H_0 admits countably many (negative) eigenvalues $(\mu_j^0)_{j\in\mathbb{N}}$, accumulating at zero.

Assertion (iii) of Theorem 3 is then proved in several steps.

Lemma 4.5.4. *For all $T \geq 0$ the map $T \mapsto i_{M,T}$ is non-decreasing and concave.*

Proof. Since β is nonnegative function, 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 $i_{M,T}$ is non-decreasing. Next, 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 $\mathcal{F}_{T_0}[\rho]$ we obtain

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

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

Remark 4.5.5. A direct consequence of the concavity of $i_{M,T}$ w.r.t. T gives rise that as $T \to T^*$ $\lim_{T\to T^*_-} i_{M,T} = 0$ assuming $T^* < +\infty$. To see this 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 (4.1.8).

Lemma 4.5.6. *There exists a $T_c > 0$ such that $i_{M,T} = i_{M,0} + T\beta(M)$ for $T \in [0, T_c]$.*

Proof. Consider a sequence $(T_n)_{n\in\mathbb{N}} \in \mathbb{R}_+$ such that $\lim_{n\to\infty} T_n = 0$. Let $\rho^{(n)} \in \mathfrak{H}_M$ denote the associated sequence of minimizers with occupation probabilities, cf. (4.5.7):

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

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

$$\mu_j^{(n)} \stackrel{n\to\infty}{\longrightarrow} \mu_j^0 \leq 0$$

where $(\mu_j^0)_{j\in\mathbb{N}}$ are the energy eigenvalues associated to H_0 as given in (4.5.8). We shall argue by contradiction and thus assume that

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

By (4.5.7) and the fact that β' is increasing, this implies: $\mu^{(n)} > \mu_1^{(n)} \stackrel{n\to\infty}{\longrightarrow} \mu_1^0$. Then

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

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. From [14], we know that this minimizer is unique and given by ρ_0, in which case

$$i_{M,T} = i_{M,0} - T\mathcal{S}[\rho_0] \equiv i_{M,0} + T\beta[M].$$

We henceforth define

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

and the assertion is proved. $\square$

As an immediate consequence of those two results we obtain the following corollary.

Corollary 4.5.7. *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 4.5.4 we conclude $i_{M,T} < i_{M,0} + T\beta(M)$ for all $T > T_c$. $\square$

We finally give an upper bound for T_c.

Proposition 4.5.8. *For $M > 0$ the critical temperature satisfies*

$$T_c \leq \frac{\mu_1^0 - \mu_0^0}{\beta'(M)}, \tag{4.5.9}$$

where $\mu_0^0 < \mu_1^0$ are the two lowest eigenvalues of H_0 defined in (4.5.8).

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 $\mu = \mu(T)$. It has to be adjusted, such that $T\beta'(M) + \mu_0^0 - \mu(T) = 0$ for any $T < T_c$ (as long as the minimizer is of rank one). This uniquely determines $\mu(T)$. On the other hand, from the Euler-Lagrange equations given in Section 4.5.2 we know

$$0 \neq \lambda_1 = (\beta')^{-1}\left(\frac{\mu(T) - \mu_1^0}{T}\right) \quad \text{if } T > \frac{\mu_1^0 - \mu_0^0}{\beta'(M)}.$$

This yields a contradiction and thus $T \leq \frac{\mu_1^0 - \mu_0^0}{\beta'(M)}$. $\square$

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- 2007, Feb 21-23: Minicourse on "Computational High Frequency Waves" by Shi Jin, WPI, Vienna, Austria
- 2007, Jul 9-14: DEASE Summerschool and Annual Meeting, WPI, Vienna, Austria
- 2007, Jul 22 - 27: Summer School "Topics in Nonlinear PDEs", CIM/UC Coimbra, Portugal
- 2008, April 7-11: Summer School "Topics and PDE's and applications 2008", FisyMat Granada, Spain
- 2008, May 5-9: Short course "Multi-scale problems and models in traffic flow", WPI, University of Vienna, Austria
- 2008, June 9-14: Summer School "Methods and Models of kinetic theory", Porto Ercole, Italy
- 2008, Sept 18-20: DEASE Summerschool and Annual Meeting, Hamburg Uni, Hamburg, Germany
- 2008, Sept 24-27: Workshop "The Gross-Pitaevskii equation and its application for BEC in optical lattices", WPI, Vienna, Austria
  Talk: "Classical limit for semi-relativistic Hartree systems"
- 2009, March 9- June 12: Supported (by IPAM) research stay at scientific program "Quantum and kinetic transport: Analysis, computations, and new applications", IPAM, UCLA, USA

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26 May, Vienna