Commun. Math. Phys. 109, 33–97 (1987)

Communications in
Mathematical
Physics

Solutions of Hartree-Fock Equations for Coulomb Systems

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Abstract. This paper deals with the existence of multiple solutions of Hartree-Fock equations for Coulomb systems and related equations such as the Thomas-Fermi-Dirac-Von Weizäcker equation.

Contents

I. Introduction

We want to present here various existence results of multiple solutions of Hartree and Hartree-Fock equations for Coulomb systems. More precisely, we consider the

* Partially supported by CEA-DAM

standard quantum description of nonrelativistic electrons interacting with static nucleii through the purely Coulombic N-body Hamiltonian,

$$H=-\sum_{i=1}^{N}\Delta_{x_i}+\sum_{i=1}^{N}V(x_i)+\sum_{i<j}\frac{1}{|x_i-x_j|}, \tag{1}$$

where

$$V(x)=-\sum_{j=1}^{m} z_j|x-\bar{x}_j|^{-1}, \quad m\geqq 1, \quad z_j>0, \quad \bar{x}_j\in\mathbb{R}^3 \quad \text{are fixed,}$$

acting on the Hilbert space $L^2(\mathbb{R}^{3N})$ or its subspace $L_a^2(\mathbb{R}^{3N})$ (consisting of functions which are antisymmetric in $x_1,\dots,x_N$). All functions will be complex-valued but everything we say below is trivially adapted to real-valued functions or complex-valued spin-dependent functions. The ground state energy is then defined by

$$E=\inf\left\{(H\Phi,\Phi)/\Phi\in H^1(\mathbb{R}^{3N})^{1}, \quad \Phi\in L_a^2(\mathbb{R}^{3N}), \quad \int_{\mathbb{R}^{3N}}|\Phi|^2\,dx=1\right\}, \tag{2}$$

with

$$(H\Phi,\Phi)=\int_{\mathbb{R}^{3N}}|\nabla\Phi|^2\,dx+\int_{\mathbb{R}^{3N}}\left\{\sum_{i=1}^{N}V(x_i)+\sum_{i<j}\frac{1}{|x_i-x_j|}\right\}|\Phi|^2. \tag{3}$$

The interpretation of this energy functional is as follows: the first term corresponds to the kinetic energy of the electrons, the second term is the 1-body attractive interaction between the electrons and the nucleii "located at $\bar{x}_j$," each of which having a total charge z_j for $1\leqq j\leqq m$, and the third term is the usual 2-body repulsive interaction between the electrons.

Because of dimensions $(3N)$, the direct computation of E seems rather hopeless and approximations are needed. Historically, the first method was introduced by Hartree [27] ignoring the antisymmetry (i.e. the Pauli principle) and choosing test functions in (2) of the form

$$\Phi(x_1,\dots,x_N)=\prod_{i=1}^{N}\varphi_i(x_i). \tag{4}$$

Later on, Fock [24] and Slater [54] proposed another class of test functions – which take into account the Pauli principle – namely the class of Slater determinants

$$\Phi(x_1,\dots,x_N)=\frac{1}{\sqrt{N!}}\sum_{\sigma}(-1)^{|\sigma|}\prod_{i=1}^{N}\varphi_{\sigma(i)}(x_i)=\frac{1}{\sqrt{N!}}\det(\varphi_i(x_j)), \tag{5}$$

where the sum is taken over all permutations σ of $\{1,\dots,N\}$ and $|\sigma|$ denotes the signature of σ. If we "restrict" the infimum in (2) to these classes of test functions, we obtain the following minimization problems

$$\operatorname{Inf}\{\mathscr{E}(\varphi_1,\dots,\varphi_N)/\varphi_i\in H^1(\mathbb{R}^3)\ \ \forall i, \quad (\varphi_1,\dots,\varphi_N)\in K\}, \tag{6}$$

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[1] $H^1(\mathbb{R}^m)=\left\{u\in L^2(\mathbb{R}^m), \frac{\partial u}{\partial x_i}\in L^2(\mathbb{R}^m) \quad \text{for all} \quad 1\leqq i\leqq m\right\}, \quad \text{for} \quad m\geqq 1$

where $\mathscr{E}$, K are given in Hartree case (4), or Hartree-Fock case (5), respectively by

$$\mathscr{E}^H(\varphi_1,\ldots,\varphi_N)=\sum_{i=1}^{N}\int_{\mathbb{R}^3}|\nabla\varphi_i|^2+V|\varphi_i|^2\,dx$$

$$+\frac{1}{2}\sum_{i\neq j}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\varphi_i|^2(x)\,\frac{1}{|x-y|}\,|\varphi_j|^2(y)\,dx\,dy, \tag{7}$$

$$K=\left\{(\varphi_1,\ldots,\varphi_N)\in L^2(\mathbb{R}^3)^N\Big/\int_{\mathbb{R}^3}|\varphi_i|^2\,dx=1\quad\text{for}\quad 1\leqq i\leqq N\right\}, \tag{8}$$

and

$$\mathscr{E}^{\mathrm{HF}}(\varphi_1,\ldots,\varphi_N)=\sum_{i=1}^{N}\int_{\mathbb{R}^3}|\nabla\varphi_i|^2+V|\varphi_i|^2\,dx \tag{9}$$

$$+\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\varrho(x)\,\frac{1}{|x-y|}\,\varrho(y)\,dx\,dy-\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{1}{|x-y|}\,|\varrho(x,y)|^2\,dx\,dy,$$

$$K=\left\{(\varphi_1,\ldots,\varphi_N)\in L^2(\mathbb{R}^3)^N\Big/\int_{\mathbb{R}^3}\varphi_i\,\varphi_j^*\,dx=\delta_{ij}\quad\text{for}\quad 1\leqq i,j\leqq N\right\}, \tag{10}$$

where z^* denotes the conjugate of the complex number z, $\varrho(x)=\sum_{i=1}^{N}|\varphi_i|^2(x)$ is the density, $\varrho(x,y)=\sum_{i=1}^{N}\varphi_i(x)\,\varphi_i^*(y)$ is the density matrix.

The Euler-Lagrange equations corresponding to Hartree problem (H in short), i.e. problem (6)–(8), are the so-called Hartree equations (H equations in short) which may be written as

$$-\Delta\varphi_i+V\varphi_i+\sum_{j\neq i}\left(|\varphi_j|^2*\frac{1}{|x|}\right)\varphi_i+\varepsilon_i\varphi_i=0\quad\text{in }\mathbb{R}^3\quad\text{for}\quad 1\leqq i\leqq N, \tag{11}$$

where $\lambda_i=-\varepsilon_i$ is the Lagrange multiplier and $(\varphi_1,\ldots,\varphi_N)\in K$. In the case of Hartree-Fock (HF) problem (6)–(9)–(10), we first observe that (9)–(10) are invariant under unitary transforms of $(\varphi_1,\ldots,\varphi_N)$, i.e. if U is a $N\times N$ unitary matrix and $(\tilde\varphi_1,\ldots,\tilde\varphi_N)=U(\varphi_1,\ldots,\varphi_N)$, then $\mathscr{E}(\tilde\varphi_1,\ldots,\tilde\varphi_N)=\mathscr{E}(\varphi_1,\ldots,\varphi_N)$ and $(\tilde\varphi_1,\ldots,\tilde\varphi_N)\in K$. Now, if $(\hat\varphi_1,\ldots,\hat\varphi_N)$ is a minimum of the HF problem, the corresponding Euler-Lagrange equations are

$$-\Delta\hat\varphi_i+V\hat\varphi_i+\left(p*\frac{1}{|x|}\right)\hat\varphi_i-\left(\int_{\mathbb{R}^3}\varrho(x,y)\,\frac{1}{|x-y|}\,\hat\varphi_i(y)\,dy\right)=\sum_j\lambda_{ij}\hat\varphi_j\quad\text{in }\mathbb{R}^3,\quad\forall i \tag{12}$$

for some hermitian matrix (λ_{ij}) of Lagrange multipliers. Hence, if we diagonalize this matrix and we use the above invariance, we find another minimum $(\varphi_1,\ldots,\varphi_N)$ solving the Hartree-Fock (HF) equations

$$-\Delta\varphi_i+V\varphi_i+\left(p*\frac{1}{|x|}\right)\varphi_i-\left(\int_{\mathbb{R}^3}\varrho(x,y)\,\frac{1}{|x-y|}\,\varphi_i(y)\,dy\right)+\varepsilon_i\varphi_i=0\quad\text{in }\mathbb{R}^3,\quad\forall i \tag{13}$$

for some $\varepsilon_i \in \mathbb{R}$ and $(\varphi_1, \ldots, \varphi_N) \in K$. In fact, D. Hartree originally derived the Hartree equations without going through the minimization procedure, and it is quite natural to look for "all" solutions of (12) or (13) (excited states), the possible minima of (6) being of course the most important ones (ground state). H and HF equations are extensively used in Atomic Physics – see for instance Hartree [28], Slater [55], Bethe and Jackiw [13], Schaeffer [51]. Notice also that very often restricted Hartree equations are considered where some of the φ_j's are taken to be equal: for example, for Helium ($m=1$, $\bar{x}_1=0$, $z_1=2$, $N=2$) one often encounters the restricted H equation which is nothing but (11) with $\varphi_1=\varphi_2$, i.e.

$$-\Delta u + Vu + \left(|u|^2 * \frac{1}{|x|}\right) u + \varepsilon u = 0 \quad \text{in } \mathbb{R}^3 \tag{14}$$

with $\varepsilon \in \mathbb{R}$, $\int_{\mathbb{R}^3} |u|^2\,dx = 1$, $Z=2$, $V(x) = -\frac{Z}{|x|}$ (for Helium).

Let us finally mention that a related equation namely the Thomas-Fermi-Von Weizäcker equation occurs in Thomas-Fermi theory (see Lieb [31, 32]; Benguria et al. [10]): this equation may be written as

$$-\Delta u + Vu + \left(|u|^2 * \frac{1}{|x|}\right) u + \lambda |u|^{p-1} u + \varepsilon u = 0 \quad \text{in } \mathbb{R}^3 \tag{15}$$

with $\varepsilon \in \mathbb{R}$, $\int_{\mathbb{R}^3} |u|^2\,dx = 1$, $p>1$, $\lambda>0$.

In this paper, we prove (in particular) the following

Theorem. *We denote by* $Z = \sum_{j=1}^{m} z_j$ *the total charge of the nucleii.*

1) *(Hartree equations). Assume* $Z > (N-1)$, *then there exists a sequence of distinct solutions* $(\varphi_1^n, \ldots, \varphi_N^n)$ $(n \geqq 1)$ *of* H *equations* (11) *such that* φ_i^n *have exponential decay at infinity and*

$$\int_{\mathbb{R}^3} |\varphi_i^n|^2\,dx = 1, \quad \textit{for all} \quad n \geqq 1,\ 1 \leqq i \leqq N.$$

2) *(Hartree-Fock equations). Assume* $Z \geqq N$, *then there exists a sequence of distinct solutions* $(\varphi_1^n, \ldots, \varphi_N^n)$ $(n \geqq 1)$ *of* HF *equations* (13) *such that*

$$\int_{\mathbb{R}^3} \varphi_i^n \varphi_j^{n*}\,dx = \delta_{ij}, \quad \textit{for all} \quad 1 \leqq i,j \leqq N,\ n \geqq 1.$$

3) *(Restricted Hartree equation). Assume* $Z \geqq 1$, *then there exists a sequence of distinct solutions* (u^n) $(n \geqq 1)$ *of* (14) *with* $\int_{\mathbb{R}^3} |u^n|^2\,dx = 1$.

4) *(*TFW *equation). Assume* $Z \geqq 1, p \geqq \frac{5}{3}$, *then there exists a sequence of distinct solutions* (u^n) $(n \geqq 1)$ *of* (15) *with* $\int_{\mathbb{R}^3} |u^n|^2\,dx = 1$.

Remarks. i) In the following sections, additional information on these solutions (regularity, exponential decay, spectral properties) will be given.

ii) It is an important open question to determine the best condition on Z (or more precisely on z_j, $\bar{x}_j$ for $1 \leqq j \leqq m$) insuring the existence of solutions of the various equations considered in the above result. In fact, best conditions (if they exist) should depend on the number of solutions one wants, the first step being best conditions for the existence of a ground state. For restricted Hartree and TFW equations it is possible to discuss the existence of a positive solution (see Benguria et al. [10] and Sect. II below).

iii) For Hartree-Fock equations, the only reference we know is the work of Lieb and Simon [37, 38] (see also Lieb [33]) where the existence of a minimum (ground state) is given requiring $Z > (N-1)$. We recall in Sect. II their method of proof and we detail some of the arguments sketched in [37]. For Hartree equations, most references we know are concerned with the existence of a positive solution (without prescribing the L^2 norm) of the restricted Hartree equation $\left(\text{with } V(x) = -\frac{Z}{|x|}\right)$ which is obtained by bifurcation or related arguments: see Reeken [51], Gustafson and Sather [26], Bazley and Seydel [7], Bazley and Zwahlen [8, 9]; Bazley et al. [6]. For the same problem, Bader [3] showed the existence of a minimum (ground state) with the normalization constraint $\left(\int_{\mathbb{R}^3} |u|^2 \, dx = 1\right)$ and Stuart [58, 59] proved the existence of infinitely many normalized solutions (by bifurcation and nodal-spectral arguments) – see also Bongers [14] for some partial results. Still for the restricted Hartree equations (and general V), we investigated in [41, 42] the existence of multiple unnormalized solutions by critical point theory arguments. Finally, J.H. Wolkowisky proved in [65] the existence of infinitely many normalized solutions of the Hartree equations in the spherically symmetric case $\left(\text{in particular } V(x) = \frac{Z}{|x|}\right)$ by a fixed point and nodal-spectral arguments.

iv) In [39], Lieb and Simon proved that the HF approximation method is asymptotically exact. □

We would like now to make a few comments on the proofs of the above theorem. In fact, even if we will give only one proof of the above theorem in its full generality, we will present below three different strategies of proofs which will give different results and two of those will work only in particular situations (basically the spherically symmetric case). These three strategies may be briefly described as follows.

1) *Direct variational, min-max critical point theory*: Here, we build convenient min-max values which yield the desired solutions through abstract results which are variations of standard results (see Rabinowitz [50], Ambrosetti and Rabinowitz [2], Berestycki and Lions [11]...), provided one checks the so-called Palais-Smale condition (a compactness condition). And this is where one encounters a non-standard difficulty: observing that we are dealing with semilinear elliptic equations which are in a vague sense sublinear (the nonlinear terms are "positive"), one sees that the only mathematical difficulty lies with the fact that one is dealing with $\mathbb{R}^3$. And, to check the Palais-Smale condition amounts to show that we can avoid the "continuous spectrum", and this happens to be equivalent to a difficult spectral

problem: one has to show that 0 cannot be an eigenvalue for a Schrödinger operator with a potential which behaves roughly speaking like a Coulomb potential at infinity. Unfortunately, this spectral problem does not seem to be solved easily and we only succeeded in showing it in the spherical symmetric situation where we can check the conditions required by a powerful result due to Agmon [1]. This approach is developed in Sects. III.1-2.

2) *Fixed point on the potential*: This approach due to Wolkowisky [65] is a mathematical version of iterative methods used for numerical purposes by physicists (successive improvements of the potential). The idea, say for problem (14) to simplify, is to consider the mapping T_k which associates to $u \in L^2(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} |u|^2\, dx \leqq 1$ the normalized eigenfunction $(T_k u)$ of the operator

$$\left[-\Delta + V + \left(|u|^2 * \frac{1}{|x|} \right) \right]$$

corresponding to the k^{th} eigenvalue, for any $k \geqq 1$ fixed. One immediately sees that this method requires in order to be meaningful to have eigenvalues of multiplicity 1; and the only way we can check this condition is by imposing spherical symmetry (see Sect. III.3). Then, under appropriate conditions one checks that T_k is well-defined and that T_k is continuous, compact and thus admits a fixed point. It would be interesting (and important for many applications) to get around the possible multiplicity of eigenvalues.

3) *Critical point theory and index bounds*: The idea is to use as in approach 1) critical point theory but to complement this by information on the index of the critical points (see Bahri [4], Viterbo [64], Bahri and Lions [5], Coffman [21] for results showing the relations between min-max critical values and indices). Then, we obtain solutions of approximated problems with a fixed upper bound on the number of negative eigenvalues of the linearized equations. This additional information (at least when $Z \geqq N$) enables us to avoid the continuous spectrum by appropriate verifications on the number of negative eigenvalues of Schrödinger type operators: in some vague sense, the spectral problem described in 1) above is replaced by a much easier spectral problem where we only have to check that certain operators have enough negative eigenvalues (verification which is also at the basis of the approach 2)). This approach is developed in Sect. IV and this is the one which enables us to prove the above theorem in full generality. Let us mention that this approach is also used to give a new proof of the existence of a ground state for Hartree and Hartree-Fock equations in Sect. II.3 (reproving thus the results of Lieb and Simon [37]).

We conclude this introduction by mentioning first that a preliminary version of the above theorem was announced in Lions [40]. Let us also point out that somewhat different Hartree-Fock equations – namely those occuring in Nuclear Physics – are studied in Gogny and Lions [25] and that we hope to come back on important variants of Hartree-Fock equations in future publications (Hartree-Fock equations with temperature in Atomic and Nuclear Physics).

To simplify notations, throughout this paper we will denote by

$$D(\varphi,\psi)=\iint_{\mathbb{R}^3\times\mathbb{R}^3}\varphi(x)\,\frac{1}{|x-y|}\,\psi(y)\,dx\,dy$$

whenever this double integral makes sense.

II. Minima

In this section we want to consider the existence of minima for the various problems described in the Introduction. In the first three sections we treat the Hartree minimization problem (6)–(8) and the Hartree-Fock minimization problem (6)–(10). We recall in Sect. II.1 the results due to Lieb and Simon [37, 38] and we present briefly a list of open questions on the existence and qualitative properties of minima. In Sect. II.2, we detail the proof of the existence of these minima (in particular because, as remarked in Lieb [34], the proof of the existence of a minimum for HF problem sketched in [37] has to be corrected and supplemented with a few details). Another reason to present this argument is to show the difference with another approach that we describe in Sect. II.3: the argument we will use there will be one of the basic tools needed to prove the existence of infinitely many solutions. Finally, in Sect. II.4 we consider variants: we first treat briefly the case of generalized restricted Hartree equations and we then consider the Thomas-Fermi-Von Weizäcker (TFW in short) equations and the Thomas-Fermi-Dirac-Von Weizäcker (TFDW in short). We will give existence results for TFW and TFDW equations which are contained in R. Benguria, H. Brézis and E. H. Lieb [10] in the case of TFW equations and which seem to be new in the context of TFDW equations. In order to do so, we will use the concentration-compactness method (Lions [43, 44]), arguments introduced in Sects. II.2–II.3 and we will need to make general observations on the concentration-compactness arguments that we develop in the Appendix.

II.1. Main Results for H *and* HF *Problems*

Theorem II.1. *Let $Z > N-1$, Then, every minimizing sequence*[2] *of the* H *problem* (6)–(8) *or of the* HF *problem* (6)–(10) *is relatively compact in* $(H^1(\mathbb{R}^3))^N$. *In particular, there exists a minimum and any minimum* $(\varphi_1, \dots, \varphi_N)$ *is (up to a unitary transform as described in the Introduction in the case of* HF *problem) a solution of* H *equations or* HF *equations.*

And in the case of the H *problem, each ε_i is the minimum eigenvalue of the operator*

$$H_i = -\Delta + V + \sum_{j\neq i}\left(|\varphi_j|^2 * \frac{1}{|x|}\right) \tag{16}$$

and $\varepsilon_i > 0$.

[2] A minimizing sequence $(\varphi_1^n, \dots, \varphi_N^n)$ is a sequence satisfying: $\mathscr{E}(\varphi_1^n, \dots, \varphi_N^n) \underset{n}{\to} \mathrm{Inf}(-)$, $(\varphi_1^n, \dots, \varphi_N^n) \in K$

In the case of the HF *problem,* $\varepsilon_1, \ldots, \varepsilon_N$ *are the N lowest eigenvalues of the operator*

$$\bar{H} = -\Delta + V + \varrho * \frac{1}{|x|} - R, \quad R\varphi = \int_{\mathbb{R}^3} \varrho(x,y) \frac{1}{|x-y|} \varphi(y)\, dy \quad \textit{for all } \varphi \in \mathscr{D}(\mathbb{R}^3) \tag{17}$$

and $\varepsilon_1, \ldots, \varepsilon_N > 0$.

Remarks. i) The fact that if a minimum exists it is a solution of H or HF equations, is standard and the study of its regularity is also standard: one shows that $\varphi_1, \ldots \varphi_N \in C_b^\infty(\mathbb{R}^3 - U)$, where U is any neighborhood of $\{\bar{x}_1, \ldots, \bar{x}_m\}$, $\varphi_1, \ldots, \varphi_N \in W^{2,p}(\mathbb{R}^3)$ for all $2 \leqq p < 3$ (in particular $\varphi_1, \ldots, \varphi_N \in C^{1,\alpha}(\mathbb{R}^3)$ for all $\alpha \in (0,1)$). In addition, if $\varepsilon_i > 0$, then φ_i has an exponential fall-off. All these properties are valid for any solution in $H^1(\mathbb{R}^3)$ of the H or HF equations (or of TFW. TFDW, restricted Hartree equations...).

ii) It is not known if the condition $Z > N - 1$ is necessary. In fact, few non-existence results seem to be known. These questions together with similar questions on the exact N-body problem are developed in Lieb [34] where it is proved that no minimum exists if $N > 2Z + m$. We also make some comments on these questions in Sect. II.3 below.

iii) All the questions related to uniqueness or non-uniqueness of minima, symmetry breakings seem to be open. For instance, if $N = 2$, is the minimum (u, v) – when it exists – of the H problem unique and thus $v \equiv u$? Even if the minimum is not unique, do we have $u \equiv v$? In the case of an atom ($\bar{x}_j = 0$ for all j), the minimization problems are invariant under orthogonal transforms of $\mathbb{R}^3$: a natural and open question is to determine when the minima have spherical symmetry or when there are symmetry breakings... If $m = 2$, similar questions may be raised with the axisymmetry around the axis $\bar{x}_1 \bar{x}_2$. For general m, we may have some particular geometric configuration of the points $\bar{x}_j$ which leads to some invariance of the H or HF minimization problems and again the possible symmetry breakings are to be investigated.

iv) The reason why we insist on the fact that all minimizing sequences are relatively compact (and thus convergent to minima up to subsequences) in the above statement is that this yields easily the orbital stability of such minima for the time-dependent H of HF equations (see Cazenave and Lions [19]). This might also be useful for numerical analysis purposes.

v) It seems important to study numerical procedures to find solutions of H and HF equations (in particular the minima). Physicists are using some iterative methods which roughly speaking correspond to build $(\varphi_1^{n+1}, \ldots, \varphi_N^{n+1})$ as the N lowest eigenfunctions (for the HF problem) of the Hamiltonian $\bar{H}^n$ obtained through the preceding configuration $(\varphi_1^n, \ldots, \varphi_N^n)$. □

We conclude this section by a few notations: we will denote by I the infimum given by (6) and we will also use the notations $I^{\mathrm{H}}, I^{\mathrm{HF}}$ to make the difference between H and HF problems when necessary. Finally, the potential V being fixed, we will denote by I_N (or $I_N^{\mathrm{H}}, I_N^{\mathrm{HF}}$) the infimum corresponding to the N-body Hamiltonian H considered in the Introduction.

II.2. Lieb-Simon's Approach

We start with a remark: the infima I^{H}, I^{HF} are also given by

$$I^{\mathrm{H}} = \mathrm{Inf}\left\{\mathscr{E}^{\mathrm{H}}(\varphi_1,\dots,\varphi_N)/\varphi_i \in H^1(\mathbb{R}^3) \quad \forall i, \quad \int_{\mathbb{R}^3} |\varphi_i|^2\,dx \leqq 1\right\}, \tag{18}$$

$$I^{\mathrm{HF}} = \mathrm{Inf}\left\{\mathscr{E}^{\mathrm{HF}}(\varphi_1,\dots,\varphi_N)/\varphi_i \in H^1(\mathbb{R}^3) \quad \forall i, \quad \left(\int_{\mathbb{R}^3} \varphi_i \varphi_j^*\,dx\right) \leqq (\delta_{ij})\right\}.^3 \tag{19}$$

This is a general observation due to the facts that the minimization problems are set in $\mathbb{R}^3$ and that $V \to 0$ as $|x| \to \infty$. We could ignore the proof of these equalities and prove Theorem II.1 as follows (in doing so we would in fact prove the equalities for $Z > N-1$) but we prefer to show them since we believe the argument involved illuminates the nature of the functionals $\mathscr{E}^{\mathrm{H}}$, $\mathscr{E}^{\mathrm{HF}}$. We prove (19) (the proof for (18) is similar and simpler): clearly we just have to prove that if $(\varphi_1,\dots,\varphi_N) \in H^1(\mathbb{R}^3)$ and $\left(\int_{\mathbb{R}^3} \varphi_i \varphi_j^*\,dx\right) \leqq (\delta_{ij})$ then $\mathscr{E}^{\mathrm{HF}}(\varphi_1,\dots,\varphi_N) \geqq I^{\mathrm{HF}}$. Indeed, let $a_{ij} = \delta_{ij} - \int_{\mathbb{R}^3} \varphi_i \varphi_j^*\,dx$, the matrix (a_{ij}) is hermitian and nonnegative. We consider $(\psi_1,\dots,\psi_N) \in \mathscr{D}(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} \psi_i \psi_j^*\,dx = a_{ij}$. By a trivial scaling argument, we may choose $(\psi_1,\dots,\psi_N)$ such that for any given $\varepsilon > 0$

$$A = \sum_{i=1}^{N} \int_{\mathbb{R}^3} |\nabla \psi_i|^2\,dx + \frac{1}{2} D(\tilde{\varrho},\tilde{\varrho}) - \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |\tilde{\varrho}(x,y)|^2 \frac{1}{|x-y|}\,dx\,dy \leqq \varepsilon, \tag{20}$$

where $\tilde{\varrho}(x) = \sum_{i=1}^{N} |\psi_i(x)|^2$, $\tilde{\varrho}(x,y) = \sum_{i=1}^{N} \psi_i(x)\psi_i^*(y)$. Let finally e_0 be any unit vector in $\mathbb{R}^3$ and let $\varphi_i^n = \varphi_i + \psi_i(\cdot + n e_0)$ for all $1 \leqq i \leqq N$. It is easy to check that

$$\int_{\mathbb{R}^3} \varphi_i^n (\varphi_j^n)^*\,dx \xrightarrow[n]{} \delta_{ij}, \quad \mathscr{E}^{\mathrm{HF}}(\varphi_1^n,\dots,\varphi_N^n) \xrightarrow[n]{} A + \mathscr{E}^{\mathrm{HF}}(\varphi_1,\dots,\varphi_N),$$

and this enables us to deduce

$$I^{\mathrm{HF}} \leqq \mathscr{E}^{\mathrm{HF}}(\varphi_1,\dots,\varphi_N) + A, \tag{21}$$

and we conclude using (20). Observe also that (18), (19) immediately yield that I^{H}, $I^{\mathrm{HF}} < 0$.

We now really begin the proof of Theorem II.1: we will do so only on the HF problem (the proof being much simpler for the H problem). There are several steps in the proof: the first one consists in showing that minimizing sequences of problem (19) are weakly convergent in H^1 to minima of (19), then one characterizes minima as convenient eigenfunctions, and one then concludes.

Step 1: *Minima of* (19). Let $(\varphi_1^n,\dots,\varphi_N^n)$ be a minimizing sequence of (19). We first check that $(\varphi_i^n)_{i,n}$ are bounded in $H^1(\mathbb{R}^3)$. To this end, we remark that by Cauchy-Schwarz inequalities we have

$$|\varrho(x,y)|^2 \leqq \varrho(x)\,\varrho(y) \quad \text{on} \quad \mathbb{R}^3 \times \mathbb{R}^3, \tag{22}$$

[3] In the sense of hermitian matrices

and we recall the following inequality which holds for all $\bar{x} \in \mathbb{R}^3$, $\varphi \in H^1(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} \frac{1}{|x-\bar{x}|} |\varphi(x)|^2 \, dx \leqq C \|\varphi\|_{L^2(\mathbb{R}^3)} \|\nabla\varphi\|_{L^2(\mathbb{R}^3)} \tag{23}$$

for some C independent of $\bar{x}$, φ. Combining these inequalities with the information that $\mathscr{E}(\varphi_1^n, \ldots, \varphi_N^n)$ is bounded from above, we deduce the H^1 bounds. Extracting if necessary a subsequence, we may assume that $\varphi_1^n, \ldots, \varphi_N^n$ converge weakly in $H^1(\mathbb{R}^3)$ and a.e. to some $\varphi_1, \ldots, \varphi_N$ which obviously satisfies

$$\left(\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx \right) \leqq (\delta_{ij}) .$$

To conclude, we check that $\mathscr{E}(\varphi_1, \ldots, \varphi_N)$ is weakly lower semi-continuous on $H^1(\mathbb{R}^3)$. In view of (22), it is easy to show that we just have to check that $\int_{\mathbb{R}^3} V|\varphi|^2 \, dx$ is weakly continuous on $H^1(\mathbb{R}^3)$ and this is a standard fact (notice for example that $V \to 0$ as $|x| \to \infty$, $V \in L^p_{\text{loc}}$ with $p > \frac{3}{2} \ldots$). Therefore, we proved that, up to subsequences, any minimizing sequence of (19) converges weakly to a minimum. To prove the existence part of Theorem II.1 we just have to show that any minimum $(\varphi_1, \ldots, \varphi_N)$ of (19) satisfies

$$\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij} \quad \forall i,j .$$

Step 2: Characterization of Minima of (19). We first observe that, since $\mathscr{E}^{\text{HF}}$ is invariant under unitary transforms of $(\varphi_1, \ldots, \varphi_N)$, we may assume that

$$\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \gamma_i \delta_{ij}, \quad \forall i,j ,$$

where $0 \leqq \gamma_i \leqq 1$. By the same argument as in the Introduction, we may also assume that $(\varphi_1, \ldots, \varphi_N)$ solve (13) for some $(\varepsilon_1, \ldots, \varepsilon_N) \in \mathbb{R}^N$. Of course, either $\varphi_i \equiv 0$, or ε_i is an eigenvalue of the Hamiltonian $\bar{H}$, for each i.

We now claim that for each i, φ_i is a minimum of

$$\operatorname{Inf} \left\{ \langle \bar{H}\varphi, \varphi \rangle / \varphi \in H^1(\mathbb{R}^3), \ \int_{\mathbb{R}^3} |\varphi|^2 \, dx \leqq 1, \ \int_{\mathbb{R}^3} \varphi \varphi_j^* \, dx = 0, \quad \forall j \neq i \right\}, \tag{24}$$

where $\langle \bar{H}\varphi, \psi \rangle$ denotes the symmetric bilinear form on $H^1(\mathbb{R}^3)$ associated with $\bar{H}$, and the value of the infimum is precisely $-\varepsilon_i \gamma_i$. Indeed, one just needs to observe that we have for each i

$$\mathscr{E}[\varphi_1, \ldots, \varphi_{i-1}, \varphi, \varphi_{i+1}, \ldots, \varphi_N] = \mathscr{E}[\varphi_1, \ldots, \varphi_{i-1}, 0, \varphi_{i+1}, \ldots, \varphi_N] + \langle \bar{H}\varphi, \varphi \rangle - Q(\varphi_i, \varphi), \tag{25}$$

where

$$Q(\varphi_i, \varphi) = D(|\varphi_i|^2, |\varphi|^2) - \operatorname{Re} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \varphi_i(x) \varphi_i^*(y) \frac{1}{|x-y|} \varphi^*(x) \varphi(y) \, dx \, dy . \tag{26}$$

Next, by Cauchy-Schwarz inequalities

$$\left| \iint_{\mathbb{R}^3\times\mathbb{R}^3} \varphi_i(x)\,\varphi_i^*(y)\,\frac{1}{|x-y|}\,\varphi^*(x)\,\varphi(y)\,dx\,dy \right|$$

$$\leqq \iint_{\mathbb{R}^3\times\mathbb{R}^3} \left\{ |\varphi_i(x)|\,\frac{1}{|x-y|^{1/2}}\,|\varphi(y)| \right\} \left\{ |\varphi_i(y)|\,\frac{1}{|x-y|^{1/2}}\,|\varphi(x)|^{1/2} \right\} dx dy$$

$$\leqq \iint_{\mathbb{R}^3\times\mathbb{R}^3} |\varphi_i(x)|^2\,\frac{1}{|x-y|}\,|\varphi(y)|^2\,dx\,dy,$$

and thus

$$Q(\varphi_i,\varphi) \geqq 0, \quad Q(\varphi_i,\varphi_i)=0. \tag{27}$$

This proves our claim on φ_i. In view of this claim, we just have to show that $\bar{H}$ admits at least N negative eigenvalues and this will imply that $(-\varepsilon_1),\dots,(-\varepsilon_N)$ are the N lowest ones (counted with multiplicity) and that $\gamma_1=\dots=\gamma_N=1$, proving thus Theorem II.1.

Step 3: *Conclusion.* We start with a general lemma (whose proof is postponed until the end of the proof of Theorem II.1).

Lemma II.1. *Let μ be a bounded nonnegative measure on $\mathbb{R}^3$ such that $\mu(\mathbb{R}^3)<Z$. Let H_1 be the Hamiltonian given by*

$$H_1 = -\Delta + V + \left(\mu * \frac{1}{|x|}\right).$$

Then H_1 admits an increasing sequence of negative eigenvalues λ_n converging to 0 as n goes to $+\infty$. □

Observing that $\bar{H} \leqq H_1$ where $\mu=\varrho(x)$, we deduce from this lemma that if one of the functions φ_i vanishes, say φ_N, then $\mu(\mathbb{R}^3)=\int_{\mathbb{R}^3}\varrho(x)\,dx=N-1$ and the condition in Theorem II.1 implies in view of the above lemma that $\bar{H}$ admits a sequence of negative eigenvalues. Therefore, $\varepsilon_1,\dots,\varepsilon_N>0$, and because of (24) we deduce a contradiction: φ_N cannot vanish since the Infimum in (24) is negative. Hence, we proved that $\gamma_1,\dots,\gamma_N>0$. Observe also that each infimum in (24) is nonpositive

$\left(\text{use for instance a standard scaling argument: } \langle \bar{H}\varphi_\sigma,\varphi_\sigma\rangle, \text{ where } \varphi_\sigma=\sigma^{-3/2}\varphi\left(\frac{\cdot}{\sigma}\right)\dots\right)$,

and thus $\varepsilon_1,\dots,\varepsilon_N \geqq 0$.

Now, if one of the constants ε_i vanishes, say ε_N, we deduce from (24) that

$$\langle \bar{H}\varphi_N,\varphi_N\rangle = 0, \ \varphi_N \not\equiv 0,$$

and thus in view of (25), (27)

$$\mathscr{E}(\varphi_1,\dots,\varphi_N)=\mathscr{E}(\varphi_1,\dots,\varphi_{N-1},0)$$

and the above analysis yields a contradiction. Therefore, $\varepsilon_1, \ldots, \varepsilon_N > 0$; $\bar{H}$ admits N negative eigenvalues; $\bar{\gamma}_1, \ldots, \bar{\gamma}_N = 1$. □

Proof of Lemma II.1. It is enough to find for each integer k a subspace of dimension k that we denote by F_k such that

$$\operatorname{Min}\left\{\langle H_1 \varphi, \varphi\rangle / \varphi \in F_k, \int_{\mathbb{R}^3} |\varphi|^2 dx = 1\right\} < 0. \tag{28}$$

To find such a F_k, we consider an arbitrary normalized $\varphi \in \mathcal{D}(\mathbb{R}^3)$ and we set $\varphi_\sigma = \sigma^{-3/2} \varphi(\cdot/\sigma)$ for $\sigma > 0$. Then we have

$$\langle H_1 \varphi_\sigma, \varphi_\sigma\rangle = \frac{1}{\sigma^2} \int_{\mathbb{R}^3} |\nabla\varphi|^2 dx + \frac{1}{\sigma} \int_{\mathbb{R}^3} V_\sigma(x) |\varphi|^2(x) + \frac{1}{\sigma} \int_{\mathbb{R}^3} \left(\mu_\sigma * \frac{1}{|x|}\right) |\varphi|^2 dx,$$

where $V_\sigma(x) = -\sum_{j=1}^{m} \frac{z_j}{|x - \bar{x}_j/\sigma|}$, $\mu_\sigma = \sigma^3 \mu(\sigma \cdot)$. In particular, if we choose φ to be radially symmetric, we may write the last term as

$$\begin{aligned}\int_{\mathbb{R}^3} \left(\mu_\sigma * \frac{1}{|x|}\right) |\varphi|^2 dx &= \int_{\mathbb{R}^3} \left(|\varphi|^2 * \frac{1}{|x|}\right) d\mu_\sigma \\ &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |\varphi(y)|^2 \max(|x|, |y|)^{-1} d\mu_\sigma(x)\, dy \\ &\leqq \int_{\mathbb{R}^3} \frac{|\varphi(y)|^2}{|y|} dy \cdot \mu_\sigma(\mathbb{R}^3) = \bar{\mu} \int_{\mathbb{R}^3} \frac{|\varphi(y)|^2}{|y|} dy,\end{aligned}$$

where $\bar{\mu} = \mu(\mathbb{R}^3)$. Now, choosing any k-dimensional space of radially symmetric functions in $\mathcal{D}(\mathbb{R}^3)$ and denoting by F_k the space obtained by rescaling them ($\varphi \to \varphi_\sigma$) as above, we obtain (28) for σ large enough. □

II.3. Another Method

First of all, we would like to make a few comments on the assumption $Z > N - 1$ and its use in the existence proofs. The potential V being fixed, we consider the sequence $(I_N)_{N \geqq 1}$ of negative numbers where I_1 is given by (one-electron ground state energy)

$$I_1 = \operatorname{Inf}\left\{\int_{\mathbb{R}^3} |\nabla\varphi|^2 + V|\varphi|^2 dx / \varphi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\varphi|^2 dx = 1\right\}. \tag{29}$$

Because of (18), (19), we obviously have

$$I_{N+1} \leqq I_N, \quad \forall N \geqq 1. \tag{30}$$

Of course, $I_1 < 0$ is achieved by a unique $\varphi_1 > 0$ on $\mathbb{R}^3$ (up to a multiplication by $e^{i\theta}$ for some $\theta \in \mathbb{R}$). And Theorem II.1 implies that if $Z > 1$ then I_2 is achieved. We now claim that even if we do not assume anything on V (or $Z, N \ldots$) we can make a few remarks on the existence of minima for the problems I_N. We now restrict our attention to HF problems (similar considerations hold in the H case). Indeed, assume that I_{N-1} is achieved for some $N \geqq 2$ at a configuration $(\varphi_1, \ldots, \varphi_{N-1})$ and that the corresponding Lagrange multipliers $\varepsilon_1, \ldots, \varepsilon_{N-1}$ are positive, i.e. the operator

$$\bar{H}_{N-1} = -\Delta + V + \varrho_{N-1} * \frac{1}{|x|} - K_{N-1}$$

admits $(N-1)$ negative eigenvalues, where $K_{N-1}\varphi = \int_{\mathbb{R}^3} \varrho_{N-1}(x,y) \frac{1}{|x-y|} \varphi(y)\, dy$ and $\varrho_{N-1}(x,y) = \sum_{i=1}^{N-1} \varphi_i(x)\varphi_i^*(y)$, $\varrho_{N-1}(x) = \sum_{i=1}^{N-1} \varphi_i(x)\varphi_i^*(x)$. Obviously, all this holds for $N=2$ ($\bar{H}_1 = -\Delta + V$). Now, consider the problem I_N: the proof given in the preceding section (in fact only some part of it) shows that only two cases may occur. Either $I_N = I_{N-1}$ and $\langle \bar{H}_{N-1}\varphi, \varphi\rangle \geqq 0$, $\forall \varphi \in H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} \varphi\varphi_i^*\, dx = 0$, $\forall i \leqq N-1$ in which case $(\varphi_1, \ldots, \varphi_{N-1}, 0)$ is a minimum of (19) and there are some minimizing sequences which are not relatively compact in H^1 or in L^2 (we do not claim that I_N is not achieved...). Or $\bar{H}_{N-1}$ admits at least N negative eigenvalues and then $I_N < I_{N-1}$, and the results stated in Theorem II.1 hold. Combining this general observation and Lemma II.1, we see that in order to prove Theorem II.1 we just need to prove it when the stronger condition $Z > N$ holds (indeed apply this case with I_{N-1} and we use the above alternative to go to I_N).

We now describe another method to prove Theorem II.1 in the case when $Z \geqq N$ for HF problems (for H problems the method below works if $Z > N-1$). To simplify the presentation, we will restrict ourselves to *real-valued* functions. The main idea of this method will be crucial for the existence theorem we stated in the Introduction. Roughly speaking, the idea of the method below is to avoid the possibility of "vanishing eigenvalues" by writing down the second minimality condition ("second derivatives have to be nonnegative at a minimum") at minima (or approximated ones). For HF problems, this condition may be written as

$$\begin{aligned}
&\sum_{i=1}^{N} \int_{\mathbb{R}^3} |\nabla\psi_i|^2 + V|\psi_i|^2 + \left(\varrho * \frac{1}{|x|}\right)|\psi_i|^2\, dx \\
&\quad - \iint_{\mathbb{R}^3\times\mathbb{R}^3} \varrho(x,y) \frac{1}{|x-y|} \psi_i(x)\psi_i(y)\, dx\, dy + \sum_{i=1}^{N} \varepsilon_i \int_{\mathbb{R}^3} |\psi_i|^2\, dx \\
&\quad + \frac{1}{2} D(K,K) - \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} |K(x,y)|^2 \frac{1}{|x-y|}\, dx\, dy \\
&\geqq 0
\end{aligned} \tag{31}$$

for all $(\psi_1, \ldots, \psi_N) \in H^1(\mathbb{R}^3)$ such that

$$\int_{\mathbb{R}^3} \psi_i\varphi_j\, dx = 0 \quad \forall i,j; \qquad \int_{\mathbb{R}^3} \psi_i\psi_j\, dx = 0 \quad \forall i \neq j, \tag{32}$$

where $K(x) = 2\left(\sum_i \varphi_i(x)\psi_i(x)\right)$, $K(x,y) = \sum_i \varphi_i(x)\psi_i(y) + \psi_i(x)\varphi_i(y)$ and ε_i are the corresponding Lagrange multipliers.

Of course, all this is a bit formal since we cannot start with a minimum and various justifications detailed below are needed. At this stage it is worth pointing out the relations between (31)–(32) and the observation (24) which was crucial for the proof given in the preceding section. In some sense, (24) is contained in (31)–(32). Indeed, for each i, we may take $\psi_j \equiv 0$ for $j \neq i$, and we deduce from (31)–(32) that for all $\psi \in H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} \psi \varphi_j \, dx = 0 \quad \forall j$,

$$\langle \bar{H}\psi, \psi\rangle + \varepsilon_i \int_{\mathbb{R}^3} |\psi|^2 dx \geqq \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \{|K(x,y)|^2 - K(x)K(y)\} \frac{1}{|x-y|} dx dy,$$

where $K(x,y) = [\varphi_i(x)\psi(y) + \psi(x)\varphi_i(y)]$, $K(x) = 2[\varphi_i(x)\psi(x)]$. But the right-hand side is nonnegative since we have

$$\tfrac{1}{4} D(K,K) = D(\varphi_i \psi, \varphi_i \psi) \quad \text{and} \quad \tfrac{1}{4} D(K,K) \leqq D(|\varphi_i|^2, |\psi|^2).$$

The way we use (31)–(32) is the following: assume to simplify that $Z > N$, then by an appropriate variant of Lemma II.1 we will show that the constants ε_i have to be bounded away from 0 and this will yield the compactness we need.

To make these vague arguments rigorous, we first claim that we can build minimizing sequences which satisfy (31)–(32) (or variants): in fact, we will see that one may assume that (31)–(32) "almost" hold for any minimizing sequence. The second step is to prove that the constants ε_i are bounded away from 0, and the final step consists in passing to the limit. We first treat the case $Z > N$ and then we explain how to modify the argument in the case when $Z = N$.

Step 1: *Minimizing Sequences and Nonnegative Hessian.* If one just wants to prove the existence of a minimum, it is easy to build *some* minimizing sequences of (6)–(10) such that (31)–(32) or close variants hold. Let us just mention two possibilities.

i) Replace $\mathbb{R}^3$ by a ball B_R of radius $R < \infty$ [i.e. set the problem (6)–(10) in the space $H_0^1(B_R)$ extending by 0 all functions of this space]. Then, the analogue of problem (6)–(10) immediately admits a minimum by standard functional analysis [use the compact embedding from $H_0^1(B_R)$ into $L^2(B_R)$]. Equations (12) for such a minimum $(\varphi_1^R, \ldots, \varphi_N^R)$ hold with $\mathbb{R}^3$ replaced by B_R and for some constants $(\varepsilon_1^R, \ldots, \varepsilon_N^R)$. Finally, (31)–(32) hold with $\mathbb{R}^3$ replaced by $B_R, \varphi_i, \varepsilon_i$ replaced by $\varphi_i^R, \varepsilon_i^R$ $(\forall i)$. Then, as $R \to \infty$, $(\varphi_1^R, \ldots, \varphi_N^R)$ is a minimizing sequence of (6)–(10).

ii) Use general optimization results: by a result due to Ekeland and Lebourg [23] (see also Ekeland [22], Stegall [56], Bourgain [15]...) we know that for all $n \geqq 1$, there exists $(f_n^i)_i \in H^{-1}(\mathbb{R}^3)$ [or even $L^2(\mathbb{R}^3)$] such that $\|f_n^i\|_{H^{-1}} \leqq 1/n$ $(\forall i)$ and there exists a minimum $(\varphi_1^n, \ldots, \varphi_N^n)$ of

$$\operatorname{Inf}\left\{\mathscr{E}^{\mathrm{HF}}(\varphi_1, \ldots, \varphi_N) - 2 \sum_{i=1}^{N} \langle f_n^i, \varphi_i\rangle / (\varphi_1, \ldots, \varphi_N) \in H^1(\mathbb{R}^3)^N, \ (\varphi_1, \ldots, \varphi_N) \in K\right\}. \tag{33}$$

Then, the Hartree-Fock equations (12) are replaced by

$$-\Delta \varphi_i^n + V\varphi_i^n + \left(\varrho^n * \frac{1}{|x|}\right)\varphi_i^n - \left(\int_{\mathbb{R}^3} \varrho^n(x,y)\varphi_i^n(y) \frac{1}{|x-y|} dy\right) + \varepsilon_i^n \varphi_i^n = f_n^i \quad \text{in } \mathscr{D}'(\mathbb{R}^3) \tag{34}$$

for some constants $(\varepsilon_1^n, \dots, \varepsilon_N^n)$, where $\varrho^n(x,y) = \sum_{i=1}^N \varphi_i^n(x)\,\varphi_i^n(y)$, $\varrho^n(x) = \varrho^n(x,x)$. And (31)–(32) hold with φ_i, ε_i replaced by $\varphi_i^n, \varepsilon_i^n$. And it is easy to check that, as n goes to ∞, $(\varphi_1^n, \dots, \varphi_N^n)$ is indeed a minimizing sequence of (6)–(10).

Unfortunately (for the reader), we are interested in the behaviour of all minimizing sequences: let $(\tilde\varphi_1^n, \dots, \tilde\varphi_N^n)$ be a minimizing sequence of (6)–(10). Then, by the general perturbation principle due to Ekeland [22], we can find another minimizing sequence $(\varphi_1^n, \dots, \varphi_N^n)$ of (6)–(10) such that

$$\|\varphi_i^n - \tilde\varphi_i^n\|_{L^2(\mathbb{R}^3)} \underset{n}{\longrightarrow} 0, \quad \forall i, \tag{35}$$

and $(\varphi_1^n, \dots, \varphi_N^n)$ is the minimum of

$$\operatorname{Inf}\left\{\mathscr{E}^{\mathrm{HF}}(\varphi_1, \dots, \varphi_N) + \delta_n \sum_{i=1}^N \|\varphi_i - \varphi_i^n\|_{L^2(\mathbb{R}^3)} / (\varphi_1, \dots, \varphi_N) \in H^1(\mathbb{R}^3)^N,\ (\varphi_1, \dots, \varphi_N) \in K\right\} \tag{36}$$

for some $\delta_n > 0$ such that $\delta_n \underset{n}{\longrightarrow} 0$. Then, "elementary" differential calculus yields the existence of $(\varepsilon_1^n, \dots, \varepsilon_N^n) \in \mathbb{R}^N$ such that the following holds

$$\begin{aligned} &-\Delta\varphi_i^n + V\varphi_i^n + \left(\varrho^n * \frac{1}{|x|}\right)\varphi_i^n - \left(\int_{\mathbb{R}^3} \varrho^n(x,y)\,\varphi_i^n(y)\,\frac{1}{|x-y|}\,dy\right) \\ &\quad + \varepsilon_i^n\,\varphi_i^n \underset{n}{\longrightarrow} 0 \quad \text{in } L^2(\mathbb{R}^3) \end{aligned} \tag{37}$$

and the existence of $\gamma^n > 0$, $\gamma^n \underset{n}{\rightarrow} 0$ such that

$$\begin{aligned} &\sum_{i=1}^N \int_{\mathbb{R}^3} |\nabla\psi_i|^2 + V|\psi_i|^2 + \left(\varrho^n * \frac{1}{|x|}\right)|\psi_i|^2 + (\varepsilon_i^n + \gamma^n)\,|\psi_i|^2\,dx \\ &\quad - \iint_{\mathbb{R}^3\times\mathbb{R}^3} \varrho^n(x,y)\,\frac{1}{|x-y|}\,\psi_i(x)\,\psi_i(y)\,dx\,dy \\ &\quad - \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} [K^n(x,y) - K^n(x)\,K^n(y)]\,\frac{1}{|x-y|}\,dx\,dy \geqq 0 \end{aligned} \tag{38}$$

for all $(\psi_1, \dots, \psi_N) \in H^1(\mathbb{R}^3)$ satisfying

$$\int_{\mathbb{R}^3} \psi_i\,\varphi_j^n\,dx = 0 \quad \forall i,j; \qquad \int_{\mathbb{R}^3} \psi_i\,\psi_j\,dx = 0 \quad \forall i \neq j, \tag{39}$$

where $K^n(x,y) = \sum_i \varphi_i^n(x)\,\psi_i(y) + \psi_i(x)\,\varphi_i^n(y)$, $K^n(x) = K^n(x,x)$. (The equality (37) just uses the differentiability on $H^1(\mathbb{R}^3)^N$ of $\mathscr{E}^{\mathrm{HF}}$ while (38) uses the fact that it is uniformly twice differentiable on bounded sets of $H^1(\mathbb{R}^3)^N$.)

Let us finally observe that these considerations are totally general and have nothing to do with HF (or H) problems.

Step 2: *Bounds from Below on* ε_i^n. This is where we use the information given by (38). To simplify the presentation, we observe that (38) implies in particular (see a similar argument above) that we have for each fixed i,

$$\int_{\mathbb{R}^3} |\nabla\psi|^2 + V|\psi|^2\,dx + \left(\varrho^n * \frac{1}{|x|}\right)|\psi|^2\,dx + (\varepsilon_i^n + \gamma^n)\int_{\mathbb{R}^3} |\psi|^2\,dx \geqq 0, \qquad (38')$$

for all $\psi \in H^1(\mathbb{R}^3)$ such that

$$\int_{\mathbb{R}^3} \psi\,\varphi_j^n\,dx = 0 \quad \forall j. \qquad (39')$$

Now, this implies that the Schrödinger operator H_n

$$-\Delta + V + \varrho^n * \frac{1}{|x|}$$

has at most N eigenvalues strictly less than $-(\varepsilon_i^n + \gamma^n)$.

For the reader's commodity, we give a simple proof of this trivial algebraic observation at the end of this step.

Now, if $Z > N$, we use Lemma II.1 and its proof to deduce that there exists $\delta > 0$ such that H_n admits for all n at least N eigenvalues strictly below $(-\delta)$. And this yields

$$\varepsilon_i^n + \gamma^n \geqq \delta.$$

Since $\gamma^n \xrightarrow[n]{} 0$, we deduce for n large enough

$$\varepsilon_i^n \geqq \varepsilon > 0, \quad \forall i. \qquad (40)$$

Lemma II.2. *Let A be a bounded, self-adjoint operator on an Hilbert space H, let H_1, H_2 be two subspaces such that $H = H_1 \oplus H_2$, $\dim H_1 = k < \infty$ and $P_2 A P_2 \geqq 0$, where P_1, P_2 denote the orthogonal projections onto H_1, H_2 respectively. Then, A has at most k negative eigenvalues.*

Remark. The assumption that A is bounded can easily be disposed of in order to accomodate the operators H_n on $L^2(\mathbb{R}^3)$.

Proof of Lemma II.2. Multiplying if necessary A by a positive constant, we may assume that $P_1 A P_1 \geqq -P_1$. Then we set $\tilde{A} = -P_1 + P_2 A P_1 + P_1 A P_2$; $\tilde{A}$ is also self-adjoint, bounded and $\tilde{A} \leqq A$. It is of course enough to show that $\tilde{A}$ has at most k negative eigenvalues. Now, if λ is an eigenvalue of $\tilde{A}$ different from 0 and if x is a corresponding eigenvector, we check easily that

$$P_2 x = \frac{1}{\lambda} P_2 A P_1 x, \; P_1 A P_2 A P_1 (P_1 x) = \lambda(\lambda + 1) P_1 x.$$

And we conclude easily observing that $P_1 A P_2 A P_1$ is a nonnegative, self-adjoint operator on H_1 and that to each eigenvalue of this operator corresponds only one negative eigenvalue of A. □

Step 3: *Conclusion.* Recalling that minimizing sequences are bounded in $H^1(\mathbb{R}^3)$, we deduce that ε_i^n is bounded, and thus we may assume (extracting subsequences if necessary) that φ_i^n converges weakly in $H^1(\mathbb{R}^3)$ (and a.e. in $\mathbb{R}^3$) to some φ_i and that ε_i^n converges to ε_i which satisfies $\varepsilon_i \geqq \varepsilon > 0$ because of (40). It is an easy exercise to pass to the limit in (37) and to recover with obvious notations

$$-\Delta\varphi_i + V\varphi_i + \left(\varrho * \frac{1}{|x|}\right)\varphi_i + \varepsilon_i\varphi_i - \int_{\mathbb{R}^3} \varrho(x,y)\,\frac{1}{|x-y|}\,\varphi_i(y)\,dy = 0. \qquad (41)$$

In particular, we find that

$$\overline{\lim_n} \sum_i \varepsilon_i^n \int_{\mathbb{R}^3} |\varphi_i^n|^2\,dx = -\underline{\lim}_n \left\{\sum_i \int_{\mathbb{R}^3} |\nabla\varphi_i^n|^2 + V|\varphi_i^n|^2\,dx \right.$$
$$\left. + \iint_{\mathbb{R}^3\times\mathbb{R}^3} \{\varrho^n(x)\,\varrho^n(y) - |\varrho^n(x,y)|^2\}\,\frac{1}{|x-y|}\,dx\,dy\right\},$$

and by the same arguments as the ones used to show that $\mathscr{E}^{\mathrm{HF}}$ is weakly lower semi-continuous on $H^1(\mathbb{R}^3)$, this yields in view of (41),

$$\overline{\lim_n} \sum_i \varepsilon_i^n \int_{\mathbb{R}^3} |\varphi_i^n|^2\,dx$$
$$\leqq -\left\{\sum_i \int_{\mathbb{R}^3} |\nabla\varphi_i|^2 + V|\varphi_i|^2\,dx + \iint_{\mathbb{R}^3\times\mathbb{R}^3} \{\varrho(x)\,\varrho(y) - |\varrho(x,y)|^2\}\,\frac{1}{|x-y|}\,dx\,dy\right\}$$
$$= \sum_i \varepsilon_i \int_{\mathbb{R}^3} |\varphi_i|^2\,dx\,.$$

Hence, φ_i^n converges strongly in $L^2(\mathbb{R}^3)$ to φ_i and it is easy to conclude the proof of Theorem II.1.

If $Z = N$, we just have to modify slightly the above argument by passing first to the limit weakly in $H^1(\mathbb{R}^3)$. Then, the operator $H = -\Delta + V + \left(\varrho * \frac{1}{|x|}\right)$ still has at most N eigenvalues less or equal than $-\varepsilon_i\,(\forall i)$, where ε_i is the limit of ε_i^n. Now, if $\int_{\mathbb{R}^3} \varrho\,dx = N$, this means that φ_i^n converges in L^2 to φ_i and the proof is over. Or $\int_{\mathbb{R}^3} \varrho\,dx < N$ and we apply Lemma II.1 to show that $\varepsilon_i > 0\ (\forall i)$: this enables us to conclude as before.

Remarks. i) If we compare the two proofs of Theorem II.1 we gave, the new one is clearly more complicated! However, the arguments we use there turn out to be crucial in Sect. II.4 for more nonlinear problems or when dealing with non-minimal solutions. In fact, the reduction from (38) to (38′) strongly uses the positivity of the Coulomb potential (as a function and as a kernel) but is not at all necessary in the above analysis provided one extends a bit Lemma II.1 (see also the next section). With this reduction the two proofs are quite parallel, but major differences can be seen on their applications (other nonlinear problems, critical points, other 2-body terms...) in particular because the reduction we did above is by no means necessary. Of course, the key point behind all the proofs is Lemma II.1 (and its extensions as we will see below).

ii) The proof in the case of Hartree minimization problems is slightly different but does not present any additional difficulty. Therefore we skip it. □

II.4. Related Minimization Problems: Restricted H, TFW, TFDW *Equations*

We begin with a generalized version of the restricted Hartree minimization problem. We consider the minimization problem (6) for the functional

$$\mathscr{E}(\varphi_1,\dots,\varphi_N)=\sum_{i=1}^{N}\int_{\mathbb{R}^3}|\nabla\varphi_i|^2+V|\varphi_i|^2\,dx+\frac{1}{2}\sum_{i,j=1}^{N}a_{ij}D(|\varphi_i|^2,|\varphi_j|^2), \tag{42}$$

and where K is given by

$$K=\left\{\varphi_i\in L^2(\mathbb{R}^3)^N\Big/\int_{\mathbb{R}^3}|\varphi_i|^2\,dx=\lambda_i\right\}, \tag{43}$$

and we assume $a_{ij}=a_{ji}\geqq 0$, $\lambda_i>0$ for all $1\leqq i,j\leqq N$.

We will call this problem the RH problem: the usual restricted problem (14) corresponds to $N=1$, $\lambda_1=1$, $a_{11}=1$ while the standard Hartree problem corresponds to $\lambda_1=\ldots=\lambda_N=1$, $a_{ij}=1-\delta_{ij}$ $\forall i,j$. We have the

Theorem II.2. *We assume that, for all* $1\leqq i\leqq N$, $\sum_j a_{ij}\lambda_j\leqq Z$ *and either* $\sum_j a_{ij}\lambda_j<Z$ *or there exists j such that* $\sum_k a_{jk}\lambda_k=Z$ *and* $a_{ji}>0$. *Then, all minimizing sequences of* (6)–(42)–(43) *are relatively compact in* $H^1(\mathbb{R}^3)$ *and in particular there exists a minimum.*

Remark. i) Of course, any minimum satisfies

$$-\Delta\varphi_i+V\varphi_i+\sum_{i=1}^{N}a_{ij}\left(|\varphi_j|^2*\frac{1}{|x|}\right)\varphi_i+\varepsilon_i\varphi_i=0\quad\text{in }\mathbb{R}^3,\quad\forall i$$

and the arguments below show that $\varepsilon_i\geqq 0$ $\forall i$. Furthermore, in general we can prove that $\varepsilon_i>0$ only if $Z>\sum_j a_{ij}\lambda_j$.

ii) If $N=1$, the condition on Z reduces to $Z\geqq\lambda_1 a_{11}$. □

Proof of Theorem II.2. We follow the arguments given in the preceding section. As in step 1, we see that we just need to consider minimizing sequences $(\varphi_1^n,\dots,\varphi_N^n)$ such that

$$-\Delta\varphi_i^n+V\varphi_i^n+\sum_{i=1}^{N}a_{ij}\left(|\varphi_j^n|^2*\frac{1}{|x|}\right)\varphi_i^n+\varepsilon_i^n\varphi_i^n\xrightarrow[n]{}0\quad\text{in }L^2(\mathbb{R}^3) \tag{44}$$

for all $i\in\{1,\dots,N\}$ and

$$\sum_{i=1}^{N}\int_{\mathbb{R}^3}|\nabla\psi_i|^2+V|\psi_i|^2+(\varepsilon_i^n+\gamma^n)|\psi_i|^2\,dx+\sum_{i=1}^{N}a_{ij}D(|\varphi_j^n|^2,|\varphi_i|^2)$$
$$-2\sum_{i,j=1}^{N}a_{ij}D(\mathrm{Re}(\varphi_i^n\psi_i^*),\mathrm{Re}(\varphi_j^n\psi_j^*)) \tag{45}$$

for some $\gamma^n > 0$, $\gamma^n \to 0$, for all $\psi_i \in H^1(\mathbb{R}^3)$ such that $\operatorname{Re} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \psi_i \varphi_i^{n*} dx = 0 \quad (\forall i)$, where ε_i^n is given by

$$\varepsilon_i^n = -\frac{1}{\lambda_i} \int_{\mathbb{R}^3} |\nabla \varphi_i^n|^2 + V|\varphi_i^n|^2 + \sum_j a_{ij} \left(|\varphi_j^n|^2 * \frac{1}{|x|} \right) |\varphi_i^n|^2 dx. \tag{46}$$

One easily checks as in Sect. II.2 that minimizing sequences are bounded in $H^1(\mathbb{R}^3)$ and thus ε_i^n is bounded $(\forall i)$. In particular, if we choose for each i fixed $\psi_j \equiv 0$ for $j \neq i$, we deduce for all $\psi \in H^1(\mathbb{R}^3)$ such that $\operatorname{Re} \int_{\mathbb{R}^3} \psi \varphi_i^{n*} dx = 0$,

$$\int_{\mathbb{R}^3} |\nabla \psi|^2 + V|\psi|^2 + (\varepsilon_i^n + \gamma^n)|\psi|^2 dx + \sum_{j=1}^N a_{ij} D(|\varphi_j^n|^2, |\psi|^2)$$
$$+ 2a_{ii} D(\operatorname{Re}(\varphi_i^n \psi^*), \operatorname{Re}(\varphi_i^n \psi^*)) \geqq 0,$$

$$H_n^i = -\Delta + V + \sum_{j=1}^N a_{ij} \left(|\varphi_j^n|^2 * \frac{1}{|x|} \right) + 2a_{ii} K_n^i$$

admits at most one negative eigenvalue (in fact using the positivity of $\frac{1}{|x|}$ as a kernel H_n^i is nonnegative), where K_n^i is defined by

$$K_n^i \varphi(x) = \left(\int_{\mathbb{R}^3} \operatorname{Re}(\varphi_i^n(y) \varphi^*(y)) \frac{1}{|x-y|} dy \right) \varphi_i^n(x), \quad \forall \varphi \in \mathcal{D}(\mathbb{R}^3).$$

To show the analogue of step 2, we will treat only the case when $Z > \sum_j a_{ij} \lambda_j$, $\forall i$ (the general case being a modification along the same lines as in the case $Z = N$ in the preceding section). In order to do so, it is clearly enough to show the following extension of Lemma II.1:

Lemma II.3. *Let μ be a bounded nonnegative measure on $\mathbb{R}^3$ such that $\mu(\mathbb{R}^3) > Z$, let $q \in L^\alpha(\mathbb{R}^3) + L^\beta(\mathbb{R}^3)$, $q \geqq 0$ with $1 < \alpha, \beta \leqq 3$ and let R be the nonnegative operator defined by*

$$Ru(x) = \left(\int_{\mathbb{R}^3} \operatorname{Re}(\psi(y) u^*(y)) \frac{1}{|x-y|} dy \right) \psi(x), \quad \forall u \in \mathcal{D}(\mathbb{R}^3),$$

where $\psi \in L^2(\mathbb{R}^3)$.

Then, for each $k \geqq 1$, there exists $\varepsilon_k > 0$ depending only on bounds on $(Z - \mu(\mathbb{R}^3))^{-1}$, q in $L^\alpha + L^\beta$, ψ in L^2 such that the operator $H = -\Delta + V + \mu * \frac{1}{|x|} + q + R$ admits at least k eigenvalues below $-\varepsilon_k$.

Remark. If $q \in L^1 + L^3$, the conclusion still holds, but ε_k depends on q. It is possible to replace $\psi \in L^2(\mathbb{R}^3)$ by $\psi \in L^r(\mathbb{R}^3) + L^2(\mathbb{R}^3)$ for some $r \in (\frac{6}{5}, 2)$.

Proof. We follow the proof of Lemma II.1 and with the same notations we find

$$\langle H\varphi_\sigma, \varphi_\sigma \rangle \leqq \frac{1}{\sigma^2} \int_{\mathbb{R}^3} |\nabla \varphi|^2 dx + \frac{1}{\sigma} \int_{\mathbb{R}^3} (V_\sigma(x) + q_\sigma(x)) |\varphi|^2 dx + \frac{\bar{\mu}}{\sigma} \int_{\mathbb{R}^3} \frac{|\varphi(y)|^2}{|y|} dy$$
$$+ \frac{1}{\sigma} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \operatorname{Re}(\psi_\sigma(y) \varphi^*(y)) \frac{1}{|x-y|} \operatorname{Re}(\psi_\sigma(x) \varphi^*(x)) dx dy,$$

where $q_\sigma(x)=\sigma q(\sigma x)$, $\psi_\sigma(x)=\sigma^{3/2}\psi(\sigma x)$. Therefore, we just need to find a k-dimensional subspace F_k of spherically symmetric functions φ in $\mathscr{D}(\mathbb{R}^3)$ such that

$$\sup_{\substack{\|\varphi\|=1\\ \varphi\in F_k}}\left[\int_{\mathbb{R}^3} q_\sigma|\varphi|^2\,dx+\iint_{\mathbb{R}^3\times\mathbb{R}^3}\operatorname{Re}(\psi_\sigma(x)\varphi^*(x))\frac{1}{|x-y|}\operatorname{Re}(\psi_\sigma(y)\varphi^*(y))\,dx\,dy\right]\to 0$$

$$\text{as}\quad \sigma\to\infty.$$

We choose an arbitrary k-dimensional subspace F_k of spherically symmetric functions φ in $\mathscr{D}(\mathbb{R}^3)$ supported say in $\{1\leqq|x|\leqq 2\}$. All norms on F_k being equivalent, we just have to show

$$\int_{1\leqq|x|\leqq 2} q_\sigma\,dx+\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\psi_\sigma(x)|\frac{1}{|x-y|}|\psi_\sigma(y)|\,1_{(1\leqq|x|\leqq 2)}\,1_{(1\leqq|y|\leqq 2)}\,dx\,dy\xrightarrow[\sigma\to\infty]{}0.$$

And we conclude since

$$\int_{1\leqq|x|\leqq 2} q_\sigma\,dx=\int_{\sigma\leqq|y|\leqq 2\sigma}\frac{1}{\sigma^2}q(y)\,dy\leqq C\left(\int_{|y|\geqq\sigma}|q|^\alpha\,dy\right)^{1/\alpha}\sigma^{3/\alpha'}\sigma^{-2}\xrightarrow[\sigma\to\infty]{}0$$

(and similarly if $q\in L^\alpha+L^\beta$) while

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\psi_\sigma(x)|\,1_{1\leqq|x|\leqq 2}\frac{1}{|x-y|}|\psi_\sigma(y)|\,1_{1\leqq|y|\leqq 2}\,dx\,dy\leqq C\left(\int_{1\leqq|x|\leqq 2}|\psi_\sigma(x)|^{6/5}\,dx\right)^{5/3}$$

$$=C\left[\sigma^{-6/5}\int_{\sigma\leqq|y|\leqq 2\sigma}|\psi(y)|^{6/5}\,dy\right]^{5/3}\leqq C\int_{\sigma\leqq|y|\leqq 2\sigma}|\psi(y)|^2\,dy,$$

and this quantity goes to 0 if $\psi\in L^2$.

To show the uniformity in q,ψ of the above construction we may argue as follows. Let q_n, ψ_n be bounded in $L^\alpha+L^3$, L^2 and assume that the k^{th} eigenvalue ε_k^n of the corresponding operator H_n goes to 0 as n goes to ∞. Without loss of generality, we may assume that q_n, ψ_n converge weakly to some $q,\psi\in L^\alpha+L^3$, L^2, and since the above construction shows that the corresponding limit operator H admits infinitely many negative eigenvalues, we reach the desired contradiction. □

Remark. If we are interested only in the existence of a minimum, it is possible to avoid the use of Lemma II.3 by building some special minimizing sequences $(\varphi_1^R,\dots,\varphi_N^R)$ as, for example, the minima of the same problem in a ball B_R, then $\varphi_1^R,\dots,\varphi_N^R>0$ on B_R by standard arguments and thus if ε_i^R are the associated Lagrange multipliesrs, the operator

$$-\Delta+V+\sum_{j=1}^N a_{ij}\left(|\varphi_j^R|^2*\frac{1}{|x|}\right)+\varepsilon_i^R$$

is nonnegative on $H_0^1(B_R)$. Then, a simple adaptation of Lemma II.1 shows that $\varepsilon_i^R\geqq\varepsilon>0$ $\left(\text{at least if }\operatorname{Max}_i\sum_{j=1}^N a_{ij}\lambda_j<Z\right)$, proving thus the compactness as in the preceding section.

However, since the above argument is not much more complicated and yields a stronger result, we prefer to emphasize the use of Lemma II.3 for we will need below the full force of Lemma II.3. □

We conclude this section by the study of a related problem: we consider the following minimization problem

$$I_\lambda = \operatorname{Inf}\left\{\mathscr{E}(u)/u \in H^1(\mathbb{R}^3),\ \int_{\mathbb{R}^3} |u|^2\,dx = \lambda\right\}, \tag{47}$$

where $\mathscr{E}$ is the functional given

$$\mathscr{E}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + Vu^2 + F(u)\,dx + \tfrac{1}{2}D(|u|^2, |u|^2), \tag{48}$$

and the functions u are taken to be real to simplify. We assume that the nonlinearity F is even, $F \in C^2(\mathbb{R}^3)$, $F(0) = F'(0) = F''(0) = 0$ and we denote by $f = F'$. Finally, in order to have a finite infimum (47) and to be able to write simply a meaningful Euler equation (and 2^{nd} order conditions)

$$F^-(t) = o(|t|^{10/3}), \quad |f'(t)| = o(|t|^4) \quad \text{as} \quad |t| \to \infty \tag{49}$$

(all these conditions are not really necessary for most of the results below but we will skip such easy extensions).

Replacing the unknown u by the density $\varrho = |u|^2$, one sees that the above minimization problem is equivalent to

$$I_\lambda = \operatorname{Inf}\left\{\int_{\mathbb{R}^3} |\nabla \varrho^{1/2}|^2 + V\varrho + F(\sqrt{\varrho})\,dx + \frac{1}{2}D(\varrho, \varrho)/\varrho \geqq 0 \right.$$
$$\left.\text{a.e.} \quad \text{in} \quad \mathbb{R}^3,\ \int_{\mathbb{R}^3} \varrho(x)\,dx = \lambda\right\}. \tag{50}$$

And when $F(s) = c|s|^{10/3}$ (with $c > 0$) – respectively $F(s) = c_1|s|^{10/3} - c_2|s|^{8/3}$ (with $c_1, c_2 > 0$) – this problem is the Thomas-Fermi-Von Weizäcker problem solved by Benguria et al. [10] – respectively the Thomas-Fermi-Dirac-Von Weizäcker problem (see Lieb [31]). These two problems occur as modified versions of the so-called Thomas-Fermi approximation of the N-body quantum problem considered in the Introduction – see Lieb [31] for further comments on the origin of these problems. Observe also that if $F \equiv 0$, (47)–(48) is nothing but the restricted Hartree problem (42)–(43) (with $N = 1$).

The fact that the infimum I_λ is finite comes from the following facts

$$\forall \varepsilon > 0,\ \exists C_\varepsilon \geqq 0,\ F^-(t) \leqq \varepsilon |t|^{10/3} + C_\varepsilon |t|^2 \tag{51}$$

and there exists $C_0 \geqq 0$ such that for all $u \in H^1(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} |u|^{10/3}\,dx \leqq C_0 \left(\int_{\mathbb{R}^3} |\nabla u|^2\,dx\right)\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)^{2/3}; \tag{52}$$

therefore

$$\mathscr{E}(u) \geqq (1 - C_0\lambda^{2/3}\varepsilon)\int_{\mathbb{R}^3} |\nabla u|^2\,dx + \int_{\mathbb{R}^3} Vu^2\,dx - C_\varepsilon\lambda.$$

This shows not only that I_λ is finite but also that minimizing sequences (u_n) are bounded in $H^1(\mathbb{R}^3)$ [and $F^+(u_n)$ are bounded in L^1].

To analyze the problem (47)–(48) we use the concentration-compactness method [43, 44]: we first introduce the problem at infinity,

$$I_\lambda^\infty = \operatorname{Inf}\left\{\mathscr{E}^\infty(u)/u \in H^1(\mathbb{R}^3),\ \int_{\mathbb{R}^3} |u|^2\,dx = \lambda\right\}, \tag{53}$$

where

$$\mathscr{E}^\infty(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + F(u)\,dx + \frac{1}{2} D(|u|^2, |u|^2). \tag{54}$$

And by the techniques of [43], we find that one always has $I_\lambda \leqq I_\alpha + I_{\lambda-\alpha}^\infty$, $\forall \alpha \in [0, \lambda]$ while the following holds.

Theorem II.3. *Every minimizing sequence of* (47)–(48) *is relatively compact in* $H^1(\mathbb{R}^3)$ *(and* $F^+(u_n)$ *is relatively compact in* $L^1(\mathbb{R}^3)$*) if and only if the following condition holds*:

$$I_\lambda < I_\alpha + I_{\lambda-\alpha}^\infty, \qquad \forall \alpha \in [0, \lambda[. \tag{S.1}$$

In particular, if (S.1) *holds, there exists a minimum of* (47)–(48).

Our goal in the remainder of this section is to give conditions which ensure that (S.1) holds. We begin by observing that if $F \geqq 0$, then one can check that $I_\lambda^\infty = 0$ for all $\lambda \geqq 0$. In fact, it is possible to generalize the condition $F \geqq 0$ as follows: we first recall that $|\nabla u|_{L^2}$ is the norm of the Hilbert space $\mathscr{D}^{1,2}(\mathbb{R}^3)$ $(= \{u \in L^2_{\text{loc}}(\mathbb{R}^3), \nabla u \in L^2(\mathbb{R}^3)\})$, while up to some irrelevant constants the norm on the dual space $(\mathscr{D}^{1,2})^*$ may be written on its dense subspace $L^{6/5}$ as

$$D(v, v)^{1/2}, \qquad \forall v \in L^{6/5}(\mathbb{R}^3)$$

[recall that $\mathscr{D}^{1,2} \hookrightarrow L^6$ and thus $L^{6/5} \hookrightarrow (\mathscr{D}^{1,2})^*$]. Therefore, there exists a constant $C_1 \geqq 0$ such that for all $u \in \mathscr{D}(\mathbb{R}^3)$,

$$\int_{\mathbb{R}^3} |u|^3\,dx \leqq C_1 \left(\int_{\mathbb{R}^3} |\nabla u|^2\,dx\right)^{1/2} \frac{1}{2} D(|u|^2, |u|^2)^{1/2}, \tag{55}$$

and we denote by C_1 the least constant such that the above inequality holds. Hence, if F satisfies

$$F(t) \geqq -\frac{2}{C_1}|t|^3 \quad \text{on} \quad \mathbb{R}, \tag{56}$$

we deduce easily $\mathscr{E}^\infty(u) \geqq 0$ and $I_\lambda^\infty \geqq 0$ for all $\lambda \geqq 0$. To check that in this case $I_\lambda^\infty = 0$, we simply consider $\varphi \in \mathscr{D}(\mathbb{R}^3)$ such that such that $\int_{\mathbb{R}^3} |\varphi|^2\,dx = \lambda$, and we compute for all $\sigma > 0$,

$$\mathscr{E}^\infty\left(\sigma^{-3/2}\varphi\left(\frac{\cdot}{\sigma}\right)\right) = \frac{1}{\sigma^2}\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx + \int_{\mathbb{R}^3} \sigma^3 F(\sigma^{-3/2}\varphi(x))\,dx + \frac{1}{2\sigma} D(|\varphi|^2, |\varphi|^2),$$

and we conclude letting σ go to $+\infty$, recalling that $F(s) = o(s^2)$.

Corollary II.1. *We assume* (56).

i) *Every minimizing sequence of* (47)–(48) *is relatively compact in* $H^1(\mathbb{R}^3)$ *if and only if*

$$I_\lambda < I_\alpha, \quad \forall \alpha \in (0, \lambda). \tag{57}$$

In particular, if (57) *holds, there exists a minimum of* (47)–(48).

ii) *There exists a constant* $\lambda_c \in (0, \infty]$ *such that for* $\lambda \leqq \lambda_c$ (57) *holds and there exists a minimum of* (47)–(48), *and for* $\lambda > \lambda_c$, λ *near* λ_c, $I_\lambda = I_{\lambda_c}$.

iii) *If* $f(t)/t$ *is nondecreasing for* $t \geqq 0$, $\lambda_c < \infty$ *and* $I_\lambda = I_{\lambda_c}$ *for* $\lambda > \lambda_c$, *and there does not exist a minimum of* (47)–(48) *for* $\lambda > \lambda_c$.

iv) *If f satisfies*

$$\forall R < \infty, \exists C_R \geqq 0, (f'(t))^+ \leqq C_R t^{2/3} \quad \textit{for} \quad 0 \leqq t \leqq R, \tag{58}$$

then $\lambda_c \geqq Z$.

Remarks. i) Part iii) of the above result corresponds to the case treated by Benguria et al. [10].

ii) In fact, it is possible to interpret Theorems II.1 and II.2 in view of the general concentration-compactness principle. For example, in Theorem II.2, denoting the infimum by $I(\lambda_1, \dots, \lambda_N)$, we observe that $I^\infty(\alpha_1, \dots, \alpha_N) = 0$ for all $\alpha_i \geqq 0$, and thus the necessary and sufficient condition given by the concentration-compactness principle reads

$$I(\lambda_1, \dots, \lambda_N) < I(\alpha_1, \dots, \alpha_N), \quad \text{for all} \quad \alpha_i \in [0, \lambda_i]$$

such that $\sum_{i=1}^N \alpha_i < \sum_{i=1}^N \lambda_i$. And the condition given in Theorem II.2 is just a condition which ensures that the above holds. Similarly for HF problems (Theorem II.1), the concentration-compactness principle yields the following necessary and sufficient condition – see Gogny and Lions [25] for related considerations –

$$I(1, \dots, 1) < I(\lambda_1, \dots, \lambda_N), \quad \text{where} \quad 0 \leqq \lambda_i \leqq 1, \ \sum_{i=1}^N \lambda_i < N,$$

where $I(\lambda_1, \dots, \lambda_N)$ corresponds to the same minimization problem with the constraints $\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \lambda_i \delta_{ij}$. Again, the condition $Z > (N-1)$ is only a condition which ensures the above strict inequality. □

Proof of Corollary II.1. Since $I_\mu^\infty = 0$ for all $\mu \geqq 0$, part i) is an immediate consequence of Theorem II.3. To prove part ii) we just have to show that (57) holds for $\lambda > 0$ small enough. To this end, we prove below that $\frac{I_\lambda}{\lambda}$ converges to

$$E_1 = \operatorname{Inf}\left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + V|u|^2 \, dx / u \in H^1(\mathbb{R}^3), \ \int_{\mathbb{R}^3} |u|^2 \, dx = 1 \right\} < 0$$

as λ goes to 0_+; and that this implies our claim on (57).

An upper bound on E_1 is easy to obtain: recall that E_1 is achieved for some $\varphi_1 > 0$ on $\mathbb{R}^3$, $\varphi_1 \in H^1(\mathbb{R}^3) \cap C_0(\mathbb{R}^3)$, and observe that

$$I_\lambda \leqq \mathscr{E}(\sqrt{\lambda}\varphi_1) \leqq \lambda E_1 + C\lambda^2 + \int_{\mathbb{R}^3} F(\sqrt{\lambda}\varphi_1)\,dx \leqq \lambda E_1 + C\lambda^2 + \lambda\varepsilon(\lambda),$$

$$\text{where} \quad \varepsilon(\lambda) \to 0 \quad \text{as} \quad \lambda \to 0_+,$$

since $F(t) = o(t^2)$ as $t \to 0$. Therefore, we have

$$\overline{\lim_{\lambda \to 0_+}} \frac{I_\lambda}{\lambda} \leqq E_1 .$$

The lower bound may be obtained by observing that (55) implies

$$\mathscr{E}(u) \geqq \int_{\mathbb{R}^3} |\nabla u|^2 + V|u|^2\,dx - \varepsilon \int_{\mathbb{R}^3} |\nabla u|^2\,dx + \frac{1}{\varepsilon} D(|u|^2, |u|^2),$$

while we have for all $\delta > 0$,

$$\begin{aligned}
&\frac{1}{\varepsilon} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|u|^2(x)\,|u|^2(y)}{|x-y|}\,dx\,dy \\
&\leqq \frac{1}{\varepsilon\delta}\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)^2 + \frac{1}{\varepsilon} \iint_{|x-y|<\delta} \frac{|u|^2(x)\,|u|^2(y)}{|x-y|}\,dx\,dy \\
&\leqq \frac{1}{\varepsilon\delta}\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)^2 + \frac{1}{\varepsilon}\left\| |u|^2 * \left(\frac{1}{|x|} 1_{|x|<\delta}\right)\right\|_{L^{3/2}} \| |u|^2 \|_{L^3} \\
&\leqq \frac{1}{\varepsilon\delta}\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)^2 + \frac{C}{\varepsilon}\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)\left\|\frac{1}{|x|} 1_{|x|<\delta}\right\|_{L^{3/2}} \cdot \left(\int_{\mathbb{R}^3} |\nabla u|^2\,dx\right) \\
&\leqq \frac{1}{\varepsilon\delta}\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)^2 + \frac{C}{\varepsilon}\delta\left(\int_{\mathbb{R}^3} |u|^2\,dx\right)\left(\int_{\mathbb{R}^3} |\nabla u|^2\,dx\right).
\end{aligned}$$

Therefore, we have for all $u \in H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} |u|^2\,dx = \lambda$,

$$\mathscr{E}(u) \geqq \left(1 - \varepsilon - \frac{C\delta}{\varepsilon}\lambda\right) \int_{\mathbb{R}^3} |\nabla u|^2\,dx + \int_{\mathbb{R}^3} V|u|^2\,dx - \frac{\lambda^2}{\varepsilon\delta},$$

and we conclude easily by convenient choices of $\varepsilon, \delta > 0$ that not only $\frac{I_\lambda}{\lambda} \to E_1$ as λ goes to 0_+ but also that if $u_\lambda \in H^1(\mathbb{R}^3)$ satisfies

$$I_\lambda \leqq \mathscr{E}(u_\lambda) \leqq I_\lambda + o(\lambda), \quad \int_{\mathbb{R}^3} |u_\lambda|^2\,dx \leqq \lambda ,$$

then $\frac{u_\lambda}{\sqrt{\lambda}}$ is a minimizing sequence of the minimization problem giving E_1, and thus (up to a change of sign) $\frac{u_\lambda}{\sqrt{\lambda}}$ converges in $H^1(\mathbb{R}^3)$ to φ_1.

To conclude the proof of our claim and thus of part ii) we claim that for all $\lambda > 0$, there exists $u_\lambda \geqq 0$ in $H^1(\mathbb{R}^3)$ such that

$$I_\lambda = \mathscr{E}(u_\lambda), \quad \int_{\mathbb{R}^3} |u_\lambda|^2\,dx \leqq \lambda . \tag{59}$$

This is another consequence of the fact that $I_\mu^\infty = 0$ for all $\mu \geqq 0$. It is deduced from the general arguments of the concentration-compactness method [43, 44]: let us just explain the basic idea behind that fact. First, observe that since $I_\lambda < 0 = I_\lambda^\infty$, if u_n is a minimizing sequence for the problem I_λ, then for some $R > 0$,

$$\int_{B_R} |u_n|^2 \, dx \geqq \delta(R) > 0$$

for some $\delta(R) > 0$ independent of n. Therefore, the only way we can lose compactness is when u_n splits in (at least) two parts: u_n^1 and u_n^2, where u_n^1 remains compact, while u_n^2 is, roughly speaking, supported outside a ball whose radius goes to ∞. Then, u_n^1 converges (in fact strongly in $H^1(\mathbb{R}^3)$) to some u_λ satisfying (59) – u_λ may also be obtained as the weak limit of u_n in L^2 or in H^1 and (59) may be deduced from careful arguments involving (55). Finally, since $I_\lambda \leqq I_\alpha$ for all $\alpha \in [0, \lambda]$, u_λ minimizes $\mathscr{E}$ on the set $\{|u|_{L^2}^2 \leqq \lambda\}$ and thus by standard arguments u_λ is of constant sign, say positive. Once the existence of u_λ is proved, the proof of ii) is easy. Indeed, by standard arguments u_λ satisfies

$$-\Delta u_\lambda + V u_\lambda + \left(|u_\lambda|^2 * \frac{1}{|x|} \right) u_\lambda + \frac{1}{2} f(u_\lambda) + \theta_\lambda u_\lambda = 0 \quad \text{in} \quad \mathbb{R}^3, \tag{60}$$

where the Lagrange multiplier θ_λ vanishes if $|u_\lambda|_{L^2}^2 < \lambda$. Furthermore, when λ goes to 0_+, we know that $\dfrac{u_\lambda}{\sqrt{\lambda}}$ converges in H^1 to φ_1 which solves

$$-\Delta \varphi_1 + V \varphi_1 = E_1 \varphi_1 \quad \text{in} \quad \mathbb{R}^3. \tag{61}$$

And this yields (to be rigorous one may use the fact that $|f(t)| \leqq \varepsilon t^2 + Ct$ for all $t \in \mathbb{R}$, $\varepsilon > 0$): $\theta_\lambda \to -E_1 > 0$ as λ goes to 0_+. Hence, for λ small enough, $\int_{\mathbb{R}^3} |u_\lambda|^2 \, dx = \lambda$.

To prove part iii), we just adapt the method of Benguria et al. [10]. Using the formula (50) and the fact that the assumption on f implies that $F(\sqrt{t})$ is convex – see also for related considerations Brézis and Oswald [18] – we see that the functional occurring in (50) is convex and that

$$I_\lambda = \operatorname{Inf} \left\{ \int_{\mathbb{R}^3} |\nabla \sqrt{\varrho}|^2 + V\varrho + F(\sqrt{\varrho}) \, dx + \frac{1}{2} D(\varrho, \varrho) / \varrho \geqq 0, \ \int_{\mathbb{R}^3} \varrho \, dx \leqq \lambda \right\}$$

is a convex function of λ. Furthermore, one checks easily that the infimum of I_λ over all $\lambda > 0$ is achieved for some (unique) ϱ_0. And, finally, $\varrho_0 \in L^1(\mathbb{R}^3)$. Setting $\lambda_c = \int_{\mathbb{R}^3} \varrho_0 \, dx$, we conclude easily, and we refer the reader to [10] for more details.

To prove part iv) we observe that if $\lambda \leqq Z$ and if $|u_\lambda|_{L^2}^2 < \lambda$ – where u_λ is the weak limit of any minimizing sequence – then $\mathscr{E}(u_\lambda) = \mathrm{I}_\lambda$, u_λ is nonnegative (up to a change of sign) and u_λ satisfies (60) with $\theta_\lambda = 0$. Finally, we have for all $\psi \in \mathscr{D}(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} |\nabla \psi|^2 + \left(V + |u_\lambda|^2 * \frac{1}{|x|} + \frac{1}{2} f'(u_\lambda) \right) |\psi|^2 \, dx + 2D(u_\lambda \psi, u_\lambda \psi) \geqq 0 \tag{61}$$

(this is nothing but the 2^{nd} order condition associated with the fact that u_λ is a local minimum of $\mathscr{E}$). We conclude using Lemma II.3 with $\mu = |u_\lambda|^2$, $q = \frac{1}{2} f'(u_\lambda)^+$,

$\psi = 2u_\lambda$: observe indeed that $u_\lambda \in C_0(\mathbb{R}^3)$ because of (60) and thus (58) implies that $q \leqq C|u_\lambda|^{2/3} \in L^3(\mathbb{R}^3)$. Then, Lemma II.3 (and its proof) contradicts (61): the contradiction shows that $|u_\lambda|^2_{L^2} = \lambda$ and this means that minimizing sequences are compact. □

Remarks. i) In part iv) of the above result, the above proof shows that $\theta_\lambda > 0$ if $\lambda < Z$.

ii) It is possible to replace (58) by

$$\forall R < \infty, \ \exists C_R \geqq 0, \ (f(t))^+ \leqq C_R t^{5/3} \quad \text{for} \quad 0 \leqq t \leqq R, \tag{58'}$$

if we use the positivity of u_λ. Indeed, u_λ being positive, (60) implies that $-\theta_\lambda$ is the lowest eigenvalue of the operator

$$-\Delta + V + |u_\lambda|^2 * \frac{1}{|x|} + \frac{1}{2}(f(u_\lambda)/u_\lambda),$$

and we can prove that $|u_\lambda|^2_{L^2} = \lambda$ as above using also Lemma II.3 and its proof. □

Before giving the last application of Theorem II.3, we want to comment a bit (56): we wish to point out that (56) excludes interesting situations like the TFDW problem and that in general I_λ^∞ does not vanish identically. For instance, if $F(t) \leqq -\frac{2k}{C_1}|t|^3$ in a neighborhood of 0 for some $k \in (0,1)$ – and this is the case for the TFDW problem – one checks that $I_\lambda^\infty < 0$ for all $\lambda > 0$. When I_λ^∞ is not identically 0, the analysis of (S.1) is much more complicated. We can prove the following

Corollary II.2. i) *The condition* (S.1) *holds for* $\lambda > 0$ *small enough, and in particular there exists a minimum for such* λ.

ii) *If* (58) *holds, then* (S.1) *holds for* $0 < \lambda \leqq Z$, *and thus there exists a minimum.*

Remarks. i) In the TFDW case, (58) holds and we have proved the existence of a minimum for $\lambda \leqq Z$.

ii) The proof of part i) above relies upon the fact that I_λ/λ converges to E_1 and I_λ^∞/λ converges to 0 as λ goes to 0_+. This enables us to use general arguments for the verification of (S.1) described in P.L. Lions [45].

iii) The proof of part ii) combines an easy extension of the arguments developed in the concentration-compactness method with the arguments developed in the preceding sections. This extension is described in the appendix – and uses in a fundamental way the fact that the Coulomb potential V decays to 0 at infinity only in a polynomial fashion, while the condition $\lambda \leqq Z$ will imply by similar considerations to those given in the preceding sections that the tentative solutions decay exponentially at infinity. In fact the condition $Z \geqq \lambda$ will also be used to "deduce that $V + |u|^2 * \frac{1}{|x|}$ is negative and decays slowly at infinity." The role of such conditions was observed in Lions [46] and the argument we use is very much related to those developed in Taubes [60, 61] and Berestycki and Taubes [12].

iv) If (58) is replaced by (58′), we still have a minimum $\lambda \leqq Z$ by an argument given above using the positivity of minima.

Proof of Corollary II.2. We first prove part i) of Corollary II.2: as we said in the remarks above, we will first show that $\frac{I_\lambda}{\lambda} \to E_1, \frac{I_\lambda^\infty}{\lambda} \to 0$ as λ goes to 0_+. The upper bound $\overline{\lim}_{\lambda \to 0_+} \frac{I_\lambda}{\lambda} \leqq E_1$ is proved exactly as in Corollary II.1 while $\overline{\lim}_{\lambda \to 0_+} \frac{I_\lambda^\infty}{\lambda} \leqq 0$, since $I_\lambda^\infty \leqq 0$. To prove the lower bound we first observe that for all $\varepsilon > 0$, there exists $C_\varepsilon \geqq 0$ such that

$$F^-(t) \leqq \varepsilon |t|^2 + C_\varepsilon |t|^{10/3} \quad \text{on } \mathbb{R}.$$

Therefore, we deduce using (52) if $|u|_{L^2}^2 = \lambda$,

$$\mathscr{E}(u) \geqq (1 - C_0 C_\varepsilon \lambda^{2/3}) \int_{\mathbb{R}^3} |\nabla u|^2 \, dx + \int_{\mathbb{R}^3} V |u|^2 \, dx - \varepsilon\lambda,$$

$$\mathscr{E}^\infty(u) \geqq (1 - C_0 C_\varepsilon \lambda^{2/3}) \int_{\mathbb{R}^3} |\nabla u|^2 \, dx - \varepsilon\lambda,$$

and the convergences of $\frac{I_\lambda}{\lambda}, \frac{I_\lambda^\infty}{\lambda}$ to E_1, 0 respectively are then easily obtained.

Next, we argue by contradiction, and we assume there exists a sequence $\lambda_n \xrightarrow[n]{} 0$ such that (S.1) does not hold for I_{λ_n}. We are going to use modifications of arguments introduced in [43]. In view of the above convergences, we may assume without loss of generality that $I_{\lambda_n} < I_{\lambda_n}^\infty$. Therefore, $\alpha_n = \inf(0 < \alpha < \lambda_n / I_{\lambda_n} = I_\alpha + I_{\lambda_n - \alpha}^\infty)$ exists and $\alpha_n > 0$. We claim that (S.1) holds for I_{α_n}. Indeed, if $I_{\alpha_n} = I_{\beta_n} + I_{\alpha_n - \beta_n}^\infty$ with $0 \leqq \beta_n < \alpha_n$, we deduce

$$I_{\lambda_n} = I_{\beta_n} + I_{\alpha_n - \beta_n}^\infty + I_{\lambda_n - \alpha_n}^\infty \geqq I_{\beta_n} + I_{\lambda_n - \beta_n}^\infty \geqq I_{\lambda_n},$$

and this contradicts the choice of α_n. Hence, there exists a minimum v_n of I_{α_n}, and we may assume that v_n is nonnegative. From the above arguments we deduce that $\frac{v_n}{\sqrt{\alpha_n}}$ converges in H^1 to φ_1, and since $\frac{I_{\lambda_n}}{\lambda_n} = \frac{\alpha_n}{\lambda_n} \frac{I_{\alpha_n}}{\alpha_n} + \left(1 - \frac{\alpha_n}{\lambda_n}\right) \frac{I_{\lambda_n - \alpha_n}^\infty}{\lambda_n - \alpha_n}$, we see that $\frac{\alpha_n}{\lambda_n} \xrightarrow[n]{} 1$. Furthermore, v_n satisfies for some $\theta_n \in \mathbb{R}$,

$$-\Delta v_n + V v_n + \left(|v_n|^2 * \frac{1}{|x|}\right) v_n + \frac{1}{2} f(v_n) + \theta_n v_n = 0 \quad \text{in} \quad \mathbb{R}^3,$$

and exactly as in the proof of Corollary II.1, the convergence of $\frac{v_n}{\sqrt{\alpha_n}}$ to φ_1 implies that θ_n converges to $(-E_1) > 0$.

To conclude, we argue as follows

$$
\begin{aligned}
I_{\lambda_n} &\leqq \mathscr{E}\left(\left(\frac{\lambda_n}{\alpha_n}\right)^{1/2} v_n\right) \\
&= I_{\alpha_n} + \left(\frac{\lambda_n}{\alpha_n} - 1\right)\left\{\int_{\mathbb{R}^3} |\nabla v_n|^2 + V|v_n|^2 + \left(|v_n|^2 * \frac{1}{|x|}\right)|v_n|^2 + \frac{1}{2} f(v_n)\, v_n\, dx\right\} \\
&\quad + \frac{1}{2}\left(\frac{\lambda_n - \alpha_n}{\alpha_n}\right)^2 \iint_{\mathbb{R}^3 \times \mathbb{R}^3} |v_n|^2(x) \frac{1}{|x-y|} |v_n|^2(y)\, dx\, dy \\
&\quad + \int_{\mathbb{R}^3} F\left(\left(\frac{\lambda_n}{\alpha_n}\right)^{1/2} v_n\right) - F(v_n) - \frac{1}{2}\left(\frac{\lambda_n}{\alpha_n} - 1\right) f(v_n)\, v_n\, dx \\
&\leqq I_{\alpha_n} - \theta_n(\lambda_n - \alpha_n) + C(\lambda_n - \alpha_n)^2 + \left(\left(\frac{\lambda_n}{\alpha_n}\right)^{1/2} - 1\right) \\
&\quad \cdot \int_0^1 \int_{\mathbb{R}^3} \left[f\left(v_n + t\left[\left(\frac{\lambda_n}{\alpha_n}\right)^{1/2} - 1\right] v_n\right) - f(v_n)\right] v_n\, dt\, dx\,,
\end{aligned}
$$

$$
I_{\lambda_n} \leqq I_{\alpha_n} - \theta_n(\lambda_n - \alpha_n) + C(\lambda_n - \alpha_n)^2 + C\frac{\lambda_n - \alpha_n}{\alpha_n}\,[\varepsilon\alpha_n + C_\varepsilon \alpha_n^3]\,,
$$

where we use the inequality $|f(t)| \leqq \varepsilon |t| + C_\varepsilon |t|^5$, hence

$$
I_{\lambda_n} \leqq I_{\alpha_n} + \frac{E_1}{2}(\lambda_n - \alpha_n)
$$

for n large enough. By assumption, this implies

$$
\frac{1}{(\lambda_n - \alpha_n)}[I_{\lambda_n} - I_{\alpha_n}] = \frac{I^\infty_{\lambda_n - \alpha_n}}{\lambda_n - \alpha_n} \leqq \frac{E_1}{2} < 0\,,
$$

contradicting the convergence of $\frac{I^\infty_\lambda}{\lambda}$ to 0 as λ goes to 0_+. The contradiction proves part i) of Corollary II.2.

We now turn to the proof of part ii) *of Corollary II.2.* We begin with the simpler case when $\lambda < Z$ to keep the ideas clear. The same argument as in Step 1 of the method described in Sect. II.3 (see also the Appendix) shows that, to analyze general minimizing sequences, it is enough to consider some particular ones (see also the Appendix) which here are sequences $(u^n)_n$ in $H^1(\mathbb{R}^3)$ satisfying

$$
\mathscr{E}(u^n) \underset{n}{\longrightarrow} I_\lambda, \quad \int_{\mathbb{R}^3} |u^n|^2\, dx = \lambda, \tag{62}
$$

$$
-\Delta u^n + Vu^n + \left(|u^n|^2 * \frac{1}{|x|}\right) u^n + \frac{1}{2} f(u^n) + \theta_n u^n \underset{n}{\longrightarrow} 0 \quad \text{in} \quad H^{-1}, \tag{63}
$$

where

$$
\theta_n = -\frac{1}{\lambda}\langle \mathscr{E}'(u^n), u^n\rangle = -\frac{1}{\lambda}\left[\int_{\mathbb{R}^3} |\nabla u^n|^2 + V|u^n|^2 + \left(|u^n|^2 * \frac{1}{|x|}\right)|u^n|^2 + \frac{1}{2} f(u^n)\, u^n\, dx\right],
$$

and for all $\psi \in H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} u^n \psi\, dx = 0$,

$$\int_{\mathbb{R}^3} |\nabla\psi|^2 + \left[V + |u^n|^2 * \frac{1}{|x|} + \frac{1}{2} f'(u^n) + (\theta_n + \gamma_n)\right] |\psi|^2\, dx$$
$$+ 2 \iint_{\mathbb{R}^3\times\mathbb{R}^3} u_n(x)\psi(x) \frac{1}{|x-y|} u_n(y)\psi(y)\, dx\, dy \geqq 0 \tag{64}$$

for some $\gamma_n \xrightarrow[n]{} 0$.

We next use (64) in conjunction with $\lambda < Z$ and (58) to deduce that θ_n (or $\theta_n + \gamma_n$) remains bounded away from 0:

$$\exists \nu > 0, \quad \theta_n \geqq \nu > 0,$$

and since u_n is bounded in $H^1(\mathbb{R}^3)$ we may assume without loss of generality that $\theta_n \xrightarrow[n]{} \theta > 0$.

And from the results of the appendix we deduce the existence of an integer $K \geqq 1$, real numbers $\alpha_1, \dots, \alpha_K$, sequences y_j^n for $2 \leqq j \leqq K$, and functions in $H^1(\mathbb{R}^3) \cap C_0(\mathbb{R}^3)$ $u_j(x)$ for $1 \leqq j \leqq K$ satisfying

$$\alpha_1 \geqq 0,\ \alpha_j > 0 \quad \text{for} \quad 2 \leqq j \leqq K,\ \sum_{j=1}^{K} \alpha_j = \lambda,\ |y_j^n| \xrightarrow[n]{} \infty \quad \text{for}$$

$$2 \leqq j \leqq K,\ |y_i^n - y_j^n| \xrightarrow[n]{} \infty \quad \text{for} \quad 2 \leqq i \neq j \leqq K,$$

$$\begin{aligned} &u^n - u_1 - \sum_{j=2}^{K} u_j(\cdot + y_j^n) \xrightarrow[n]{} 0 \quad \text{in} \quad H^1(\mathbb{R}^3),\ \int_{\mathbb{R}^3} |u_j|^2\, dx = \alpha_j,\\ &\mathscr{E}(u_1) = I_{\alpha_1},\ \mathscr{E}^\infty(u_j) = I_{\alpha_j}^\infty \quad \text{for} \quad 2 \leqq j \leqq K,\ I_\lambda = I_{\alpha_1} + \sum_{j=2}^{K} I_{\alpha_j}^\infty,\\ &-\Delta u_1 + V u_1 + \left(|u_1|^2 * \frac{1}{|x|}\right) u_1 + \frac{1}{2} f(u_1) + \theta u_1 = 0 \quad \text{in} \quad \mathbb{R}^3,\\ &-\Delta u_j + \left(|u_j|^2 * \frac{1}{|x|}\right) u_j + \frac{1}{2} f(u_j) + \theta u_j = 0 \quad \text{in} \quad \mathbb{R}^3,\ 2 \leqq j \leqq K. \end{aligned} \tag{65}$$

Of course if $\alpha_1 = \lambda$, then the compactness is proved, and to prove that (S.1) holds we are going to show that such a decomposition of I_λ with minima satisfying the Euler equations with the *same* Lagrange multiplier is not possible. Before going into this final argument, we would like to comment on the information given in (65): the concentration-compactness arguments yield in fact the decomposition of a minimizing sequence in a finite number of pieces converging to minima of subproblems as before, the only new information comes from the Euler equations satisfied by those minima. Indeed, all the minima share the same Lagrange multiplier θ which is of course the limit of θ_n, the Lagrange multiplier occurring in (63). In fact, we will not use here the full force of this decomposition since we will only use the fact that this implies that all the Lagrange multipliers associated with u_j are strictly positive (if we were able to prove directly this fact, we would not need such a precise decomposition). However, the full information may be crucial on other problems. Let us finally mention that related decompositions (with different types of lack of compactness) were investigated by Sacks and Uhlenbeck [52], Uhlenbeck [62, 63], Brézis and Coron [16], Struwe [57]....

We may now conclude the proof of Corollary II.2: the idea is simple, we take K points $e_j (1 \leqq j \leqq K)$ such that $e_1 = 0$, $|e_j| = 1$ for $j \geqq 2$, $|e_i - e_j| > 0$ if $i \neq j$, and we consider $w_t = u_1 + u_2(x + e_2 t) + \sum_{j=3}^{K} u_j(x + e_j t^2)$, $v_t = \frac{w_t}{|w_t|_{L^2}} \sqrt{\lambda}$ for $t \geqq 0$. By definition $I_\lambda \leqq \mathscr{E}(v_t)$ while $|v_t|_{L^2}^2 = \lambda$. Since we have easily

$$|w_t|_{L^2}^2 \xrightarrow[t \to +\infty]{} \lambda, \ \mathscr{E}(v_t), \ \mathscr{E}(w_t) \xrightarrow[t \to +\infty]{} I_{\alpha_1} + \sum_{i=2}^{K} I_{\alpha_i}^{\infty} = I_\lambda,$$

if we prove that for t large, $\mathscr{E}(v_t) < I_{\alpha_1} + \sum_{j=2}^{K} I_{\alpha_j}^{\infty}$, we reach a contradiction which proves part ii) of Corollary II.2. To investigate the behaviour of $\mathscr{E}(v_t)$ for t large, we first remark that since $f'(0) = 0$ we deduce from (65) by standard arguments that for every $v \in (0, \theta^{1/2})$ there exists a constant $C \geqq 0$ such that

$$|\nabla u_j(x)| + |u_j(x)| \leqq C \exp(-v|x|) \quad \text{for} \quad |x| \geqq R, \tag{66}$$

where $R > \max_{1 \leqq j \leqq m} |\bar{x}_j|$. In particular, this implies

$$\lambda \leqq |w_t|_{L^2}^2 = \lambda + 2 \sum_{1 \leqq i < j \leqq K} \int_{\mathbb{R}^3} u_i u_j \, dx \leqq \lambda + C \exp(-vt)$$

for some $C \geqq 0$ depending only on $v \in (0, \theta^{1/2})$. Therefore, we deduce easily

$$v_t = \lambda(t) w_t, \quad |\lambda(t) - 1| \leqq C \exp(-vt)$$

and

$$|\mathscr{E}(v_t) - \mathscr{E}(w_t)| \leqq C \exp(-vt).$$

Next, we claim that

$$\mathscr{E}(v_t) = \mathscr{E}(u_1) + \sum_{j=2}^{K} \mathscr{E}^\infty(u_j) + \frac{1}{t}\{\alpha_1 \alpha_2 - Z\alpha_2\} + o\left(\frac{1}{t}\right), \quad \text{as} \quad t \to +\infty. \tag{67}$$

At this point, we just observe that in view of (65), $\mathscr{E}(u_1) = I_{\alpha_1}$, $\mathscr{E}(u_j) = I_{\alpha_j}^\infty$ for $2 \leqq j \leqq K$ and since $Z \geqq \lambda = \sum_{i=1}^{K} \alpha_i$, we have proved the desired behaviour of $\mathscr{E}(v_t)$, and we may conclude.

Hence, it just remains to prove (67). Using (66) one obtains in a straightforward way denoting by $\tilde{u}_1 = u_1$, $\tilde{u}_2 = u_2(\cdot + e_2 t)$, $\tilde{u}_j = u_j(\cdot + e_j t^2)$ for $j \geqq 3$

$$\begin{aligned} \mathscr{E}(v_t) = \mathscr{E}(u_1) &+ \sum_{j=2}^{K} \mathscr{E}^\infty(u_j) + \sum_{j=2}^{K} \int_{\mathbb{R}^3} V(x) |\tilde{u}_j|^2 \, dx \\ &+ \sum_{1 \leqq i < j \leqq K} D(|\tilde{u}_i|^2, |\tilde{u}_j|^2) \\ &+ o(\exp - vt) + \int_{\mathbb{R}^3} \left\{ F(v_t) - \sum_{j=1}^{K} F(\tilde{u}_j) \right\} dx. \end{aligned}$$

We first bound the last term: we have for t large enough

$$\left|\int_{\mathbb{R}^3}\left\{F(v_t)-\sum_{j=1}^{K}F(\tilde{u}_j)\right\}dx\right| \leqq \sum_{j=1}^{K}\int_{|x+e_j(t)|\leqq t/2}|F(v_t)-F(\tilde{u}_j)|\,dx$$

$$+\int_{\cap(|x+e_j(t)|>t/2)}|F(v_t)|+\sum_{j=1}^{K}|F(\tilde{u}_j)|\,dx,$$

where $e_1(t)=0$, $e_2(t)=te_2$, $e_j(t)=t^2e_j$ for $j\geqq 3$.

Each term in the sum may be bounded by

$$\int_{|x+e_j(t)|\leqq t/2}\left\{\sum_{j=1}^{K}|\tilde{u}_j|+C\sum_{j=1}^{K}|\tilde{u}_j|^5\right\}\left(\sum_{i\neq j}\tilde{u}_i\right)dx\leqq C\exp(-\nu t),$$

while the last integral is easily bounded by

$$C\int_{\cap(|x+e_j(t)|>t/2)}|v_t|^2+\sum_{j=1}^{K}|\tilde{u}_j|^2\,dx\leqq C\exp(-\nu t).$$

To conclude, we just have to prove

$$\int V|\tilde{u}_2|^2\,dx=\frac{-Z\alpha_2}{t}+o\left(\frac{1}{t}\right),$$

$$\int V|\tilde{u}_j|^2\,dx=\frac{-Z\alpha_j}{t^2}+o\left(\frac{1}{t^2}\right)\qquad\text{for}\quad j\geqq 3\quad\text{as}\quad t\to\infty,$$

$$D(|\tilde{u}_j|^2,|\tilde{u}_j|^2)=\frac{\alpha_i\alpha_j}{|e_i-e_j|\,t^2}+o\left(\frac{1}{t^2}\right)\qquad\text{for}\quad i\neq j\geqq 3,$$

$$D(|u_1|^2,|\tilde{u}_j|^2)=\frac{\alpha_1\alpha_j}{t^2}+o\left(\frac{1}{t^2}\right)\qquad\text{for}\quad j\geqq 3,$$

$$D(|u_1|^2,|\tilde{u}_2|^2)=\frac{\alpha_1\alpha_2}{t}+o\left(\frac{1}{t}\right),$$

$$D(|\tilde{u}_2|^2,|\tilde{u}_j|^2)=\frac{\alpha_2\alpha_j}{t^2}+o\left(\frac{1}{t^2}\right)\qquad\text{for}\quad j\geqq 3.$$

All these equalities are simple consequences of the following observations

$$|z|\int_{\mathbb{R}^3}\frac{1}{|x-z|}|u(x)|^2\,dx\xrightarrow[|z|\to\infty]{}\int_{\mathbb{R}^3}|u(x)|^2\,dx,$$

$$|z|\iint_{\mathbb{R}^3\times\mathbb{R}^3}|u(x)|^2|v(y)|^2\frac{1}{|x-y-z|}\,dx\,dy\xrightarrow[|z|\to\infty]{}\left(\int_{\mathbb{R}^3}|u(x)|^2\,dx\right)\cdot\left(\int_{\mathbb{R}^3}|v(y)|^2\,dy\right)$$

which hold for general $u, v\in H^1(\mathbb{R}^3)\cap C_0(\mathbb{R}^3)$ provided u, v "decay fast enough at infinity", in particular if u, v decay exponentially at infinity as it is the case here.

Next, we have to explain why (62)–(64) imply that θ_n remains bounded away from 0 even in the case when $Z=\lambda$ if u^n is not compact. Indeed, we may assume that u^n is not relatively compact in $L^2(\mathbb{R}^3)$ and this means (up to subsequences) that u^n converges weakly in $H^1(\mathbb{R}^3)$ and a.e. to some u such that $\int_{\mathbb{R}^3}|u|^2\,dx=\alpha<\lambda$. Then,

$|u^n|^2$ converges weakly in the sense of measures (and in L^3) to $|u|^2$ and $f'(u^n)$ converges weakly in $L^3+L^{3/2}$ (for example) to $f'(u)$. Next, we observe that the operator $-\Delta+V+|u|^2*\frac{1}{|x|}+\frac{1}{2}f'(u)+2K_0$ with $K_0\varphi=\left[(u\varphi)*\frac{1}{|x|}\right]u$ admits in view of Lemma II.3 infinitely many negative eigenvalues. And if $\theta_n^+\xrightarrow[n]{}0$, we reach easily a contradiction with (64).

Let us finally mention that (58) is basically optimal since one can show (see Léon [30]) that for any $1<q<\frac{5}{3}$ and for any $Z>0$ there exists a constant $C(z)$ (going to 0 as $Z\to 0$) such that any solution v of

$$-\Delta v-\frac{Z}{|x|}v+|v|^{q-1}v+\lambda v=0 \quad \text{in } \mathbb{R}^3, \quad v\in L^2_{\text{loc}}(\mathbb{R}^3)$$

for some $\lambda\geqq 0$, satisfies $\int_{\mathbb{R}^3}|v|^2\,dx\leqq C(z)$. Related results obtained previously may be found in Lieb [35], Lieb and Liberman [36]. On the other hand, the above arguments yield the existence of a positive solution of this equation with $\int_{\mathbb{R}^3}|v|^2\,dx$ arbitrary when $q\geqq\frac{5}{3}$.

III. Partial Existence Results

Our goal in this section is to present two methods – which were briefly described in the Introduction – which do not seem to yield the same generality of results as the method introduced in Sect. IV. The first method relies on some easy critical point results where some compactness condition, namely the Palais-Smale (P.S.) condition, is assumed to hold: these results are given in Sect. III.1. The application to H problems is given in Sect. III.2. And finally in Sect. III.3 we consider a fixed a fixed point approach (2nd approach described in the Introduction). These two approaches seem to work only in the spherically symmetric situation.

III.1. Some Abstract Critical Point Results

Let E be an infinite dimensional Banach space and let H be an infinite dimensional Hilbert space; its dual space H^* is identified with H and we assume that E is continuously embedded into H. We denote by $\|\cdot\|$ the norm on E, $\|\cdot\|_*$ the norm on E^*, $|\cdot|$ the norm on H and $(\cdot,\cdot)$ the scalar product in H. Let $N\geqq 1$, we denote by M_{H}, M_{HF} the following manifolds:

$$M_{\mathrm{H}}=\{u=(u_1,\dots,u_N)\in E^N/|u_i|=1 \quad \text{for all} \quad 1\leqq i\leqq N\}, \tag{68}$$

$$M_{\mathrm{HF}}=\{u=(u_1,\dots,u_N)\in E^N/(u_i,u_j)=\delta_{ij} \quad \text{for all} \quad 1\leqq i,j\leqq N\}. \tag{69}$$

And we consider an even C^1 functional $\mathscr{E}$ on E^N. We will need a few more notations: we denote by Σ_{H} (respectively Σ_{HF}) the collection of all compact symmetric sets included in M_{H} (respectively M_{HF}), Γ^k_{H} (respectively Γ^k_{HF}) the collection of all sets A in Σ_{H} (respectively Σ_{HF}) whose genus is more than k, i.e.

$$\gamma(A)=\inf\{j\geqq 1/\exists h \text{ odd, continuous from } A \text{ into } S^{j-1}\}\geqq k \quad [4]$$

[4] For the main properties of the genus, we refer to Krasnosel'skii [29], Rabinowitz [50], Ambrosetti and Rabinowitz [2]

and Θ_{H}^k (respectively Θ_{HF}^k) the collection of all odd continuous maps from S^{k-1} into M_{H} (respectively M_{HF}). Here and below k denotes some integer ($k \geqq 1$). We then introduce two sequences of values, which at this stage are possibly infinite,

$$b^k = \inf_{A \in \Gamma^k} \max_{u \in A} \mathscr{E}(u), \quad \forall k \geqq 1 \tag{70}$$

$$c^k = \inf_{h \in \Theta^k} \max_{\xi \in S^{k-1}} \mathscr{E}(h(\xi)), \quad \forall k \geqq 1 \tag{71}$$

and, when needed, b_{H}^k, b_{HF}^k, c_{H}^k, c_{HF}^k will correspond obviously to the H of HF choices. Notice also that if $h \in \Theta^k$, then $\gamma(h(S^{k-1})) \geqq k$, therefore

$$b^k \leqq c^k, \quad \forall k \geqq 1. \tag{72}$$

Finally, we will say that $\mathscr{E}$ satisfies (P.S.-c) on M_{H} (respectively M_{HF}) where $c \in \mathbb{R}$ if the following condition holds:

$$\begin{gathered}\text{for each sequence } u^n \text{ in } M_{\mathrm{H}} \text{ (respectively } M_{\mathrm{HF}}) \text{ such that}\\ \mathscr{E}(u^n) \xrightarrow[n]{} c \text{ and } (\mathscr{E}|_{M_{\mathrm{H}}})'(u^n) \xrightarrow[n]{} 0 \text{ in } E^{N*} \text{ (respectively}\\ (\mathscr{E}|_{M\mathrm{HF}})'(u^n) \xrightarrow[n]{} 0 \text{ in } E^{N*}) \text{ then } u^n \text{ is relatively compact in } E^N.\end{gathered} \tag{73}$$

Then, we have the

Theorem III.1. *Assume that $\mathscr{E}$ is bounded from below on M_{H} (respectively M_{HF}).*

1) *Let $k \geqq 1$. If $\mathscr{E}$ satisfies* (P.S.-b^k) *or* (P.S.-c^k) *on M_{H} (respectively M_{HF}) then b^k or c^k is a critical value of $\mathscr{E}$ on M_{H} (respectively M_{HF}).*

2) *Assume that E is separable and dense into H, that $b^k < \mathscr{E}(0)$ for all $k \geqq 1$ and and that $\mathscr{E}$ satiesfies the following condition*:

$$\begin{gathered}\textit{for each sequence } v^k \textit{ in } M_{\mathrm{H}} \textit{ (respectively } M_{\mathrm{HF}}) \textit{ such that } \mathscr{E}(v^k) < \mathscr{E}(0)\\ \textit{for all } k \geqq 1 \textit{ and } v^k \to 0 \textit{ weakly in } H^N, \textit{ then } \varliminf_k \mathscr{E}(v^k) \geqq \mathscr{E}(0)\end{gathered} \tag{74}$$

then $b^k \uparrow \mathscr{E}(0)$ as $k \uparrow +\infty$.

Remarks. i) We will need part 2) of the above result in Sect. IV.

ii) These results are variants and adaptions of results given in Berestycki and Lions [11].

iii) As usual, if $b^k = b^{k+1} = \ldots = b^{k+r}$ for some $r \geqq 1$ then the genus of the critical points associated with b^k [we assume of course that (P.S.) holds] is more than $r+1$.

iv) If in (73) u^n is bounded in E^N, then the condition

$$(\mathscr{E}|_{M_{\mathrm{H}}})'(u^n) \xrightarrow[n]{} 0 \quad \text{in} \quad E^{N*} \quad \text{or} \quad (\mathscr{E}|_{M_{\mathrm{HF}}})'(u^n) \xrightarrow[n]{} 0 \quad \text{in} \quad E^{N*}$$

is equivalent to

$$\mathscr{E}_i'(u^n) - \langle \mathscr{E}_i'(u^n), u_i^n \rangle u_i^n \xrightarrow[n]{} 0 \quad \text{in} \quad E^*, \quad \forall 1 \leqq i \leqq N$$

or

$$\mathscr{E}_i'(u^n) - \sum_{j=1}^N \langle \mathscr{E}_i'(u^n), u_j^n \rangle u_j^n \xrightarrow[n]{} 0 \quad \text{in} \quad E^*, \quad \forall 1 \leqq i \leqq N.$$

We will only sketch the proof of Theorem III.1 since it is an easy adaption of the corresponding proofs in Berestycki and Lions [11]; and, of course, these schemes of proofs originate from Ljusternik and Schnirelman [47], Palais [48, 49], Clarke [20], Rabinowitz [50], Ambrosetti and Rabinowitz [2]....

The proof of part 1) is a standard deformation argument: some attention has to be paid to the fact we are dealing with two spaces E, H but this is solved exactly as in [11], and also to the fact that we have multiple constraints in the definitions of M_{H}, M_{HF}. This second difficulty is also solved as in [11] by building a pseudo-gradient vector field $v(x)$, i.e. a mapping from M_{H} (respectively M_{HF}) into $T(M_{\mathrm{H}})$ (respectively $T(M_{\mathrm{HF}})$) which is locally Lipschitz on the complement of critical points of $\mathscr{E}|_{M_{\mathrm{H}}}$ (respectively $\mathscr{E}|_{M_{\mathrm{HF}}}$) and such that for all $u \in M_{\mathrm{H}}$ (respectively M_{HF}), $v(u) \in T_u(M_{\mathrm{H}})$ (respectively $T_u(M_{\mathrm{HF}})$), i.e. $v(u) \in E$ and

$$\forall 1 \leqq i \leqq N \qquad (v_i(u), u_i)_{\mathrm{H}} = 0 \qquad \text{in the case of } M_{\mathrm{H}}$$

$$\forall 1 \leqq i, j \leqq N \qquad (v_i(u), u_j)_{\mathrm{H}} = 0 \qquad \text{in the case of } M_{\mathrm{HF}}$$

and $v(u)$ satisfies

$$\|v(u)\|_E \leqq 2 \|(\mathscr{E}|_{M_{\mathrm{H}}})'(u)\| \qquad (\text{respectively } \|(\mathscr{E}|_{M_{\mathrm{HF}}})'(u)\|)$$

$$\langle (\mathscr{E}|_{M_{\mathrm{H}}})'(u),\ v(u)\rangle \geqq \|(\mathscr{E}|_{M_{\mathrm{H}}})'(u)\|^2$$

replacing obviously M_{H} by M_{HF} in the other situation. The remainder of the proof follows the one in [11].

To prove part 2) we consider a nested sequence E_k of finite dimensional subspaces of E^N such that $\bigcup_{k \geqq 1} E_k$ is dense in E^N and thus in H^N and $\dim E_k = k$. Then, for each $k \geqq 1$, we choose $A \in \Gamma^k$ such that

$$b^k \leqq \max_{u \in A} \mathscr{E}(u) \leqq \frac{\mathscr{E}(0) + b^k}{2}. \tag{75}$$

Next, we consider the space $F_k = E_{k-1}^{\perp}$ (orthogonal complement of E_{k-1} in H). It is standard that $F_k \cap A \neq \emptyset$: we recall the argument since we are dealing with two different spaces E^N, H^N. By way of contradiction, assume that $F_k \cap A = \emptyset$, then denoting by π_{k-1} the orthogonal projection in H^N onto E_{k-1} we deduce that

$$\pi_{k-1}(A) \subset E_{k-1} - \{0\}.$$

And since π_{k-1} is continuous on E^N and obviously odd we reach a contradiction with the choice of A in Γ^k.

Hence, there exists v^k in $F_k \cap A$: because of (75), $\mathscr{E}(v^k) < \mathscr{E}(0)$, and obviously $v^k \in M$, $v^k \to 0$ weakly in H^N. Therefore, $\underline{\lim}_k\, \mathscr{E}(v^k) \geqq \mathscr{E}(0)$ by assumption (74) and we conclude since

$$\mathscr{E}(v^k) \leqq \frac{\mathscr{E}(0) + b^k}{2}, \qquad b^k < \mathscr{E}(0).$$

III.2. Application to Hartree Equations

We want now to apply the above results to the simplest example of the restricted Hartree equation (14), i.e. we take $E=H^1(\mathbb{R}^3)$, $H=L^2(\mathbb{R}^3)$, $N=1$, and

$$\mathscr{E}(\varphi)=\int_{\mathbb{R}^3}|\nabla\varphi|^2+V|\varphi|^2\,dx+\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\varphi|^2(x)\,|\varphi|^2(y)\,\frac{1}{|x-y|}\,dx\,dy.$$

Since $\mathscr{E}$ is bounded from below on M_{H}, we just need to check (P.S.-b^k) or (P.S.-c^k), that $b^k<\mathscr{E}(0)=0$ and that (74) holds. As we will see below the main difficulty lies with (P.S.) that we are only able to check in the spherically symmetric situation, i.e. $\bar{x}_j\equiv 0$ for all j. And furthermore we will only consider radial functions $\varphi(x)=\varphi(|x|)$, i.e. we will work with

$$\begin{aligned}E&=H_r^1(\mathbb{R}^3)=\{\varphi\in H^1(\mathbb{R}^3)/\varphi(x)=\varphi(|x|)\}\\ H&=L_r^2(\mathbb{R}^3)=\{\varphi\in L^2(\mathbb{R}^3)/\varphi(x)=\varphi(|x|)\}.\end{aligned}\tag{76}$$

With these notations, we have the

Theorem III.2.

1) *If* $E=H^1(\mathbb{R}^3)$, $H=L^2(\mathbb{R}^3)$, *then* $b^k\leqq c^k<0$ *and* (74) *holds.*

2) *Assuming that* $\bar{x}_j\equiv 0$ *for all* j, $Z\geqq 1$ *and taking* E, H *as in* (76), *then the new values* b^k, c^k *still satisfy* $b^k\leqq c^k<0$ *and* (74) *holds. Furthermore,* $\mathscr{E}$ *satisfies* (P.S.-c) *on* M_{H} *for all* $c<0$.

Before proving Theorem III.2, we give the following

Corollary III.1. *If we assume* $Z\geqq 1$ *and* $\bar{x}_j\equiv 0$ *for all* j, *and if we take* E, H *as in* (76), *then the values* b^k, c^k *are critical values and* $b^k\underset{k}{\uparrow}0$, $c^k\underset{k}{\uparrow}0$. *To each critical value corresponds at least one solution* φ^k *of the restricted Hartree equation* (14) *such that* $|\varphi^k|_{L^2(\mathbb{R}^3)}=1$ *for all* $k\geqq 1$, φ^k *is radial, the Lagrange multiplier* ε^k *in* (14) *is nonnegative and if* $Z>1$ *it is positive and thus* φ^k *decays exponentially fast at infinity. Finally, as* k *goes to* ∞, φ^k *converges to* 0 *in* $L^p(\mathbb{R}^3)$ (*for* $2<p\leqq\infty$), $\nabla\varphi^k$ *converges to* 0 *in* $L^2(\mathbb{R}^3)$ *and* ε^k *converges to* 0.

Remarks. 1) It is possible to treat by the same method some equations like TFW equations but the unnecessary (in view of Sect. IV) restrictions on the nonlinearities make such statements almost useless.

2) At least for scalar problems, we will see below that the main difficulty lies with the (P.S.) condition and that, for instance, we would be able to treat by similar arguments the general restricted equation (14) without restricting V to be $-\frac{Z}{|x|}$ as we do above provided one could answer positively the following question: let $\varrho\in L_+^1(\mathbb{R}^3)$ be such that $\varrho=|v|^2$ with $v\in H^1(\mathbb{R}^3)$ and let $u\in H^1(\mathbb{R}^3)$ be a solution of

$$-\Delta u+Vu+\left(\varrho*\frac{1}{|x|}\right)u=0\quad\text{in}\quad\mathbb{R}^3.$$

Then, does the condition $Z>\int_{\mathbb{R}^3}\varrho\,dx$ imply $u\equiv 0$?

3) In fact, the above result also yields the existence of infinitely many solutions for the general Hartree equations (11) provided $Z \geqq (N-1)$ (and if $Z > N-1$ the multipliers $\varepsilon_i^k > 0$). Indeed, observe first that by a simple scaling we may replace the constraint $\int_{\mathbb{R}^3} |\varphi|^2\,dx = 1$ by $\int_{\mathbb{R}^3} |\varphi|^2\,dx = \lambda$, where $\lambda > 0$ and the above result holds if $Z \geqq \lambda$. Then, if we choose for all $1 \leqq i \leqq N$, $\varphi_i^k = \frac{1}{\sqrt{N-1}}\varphi^k$ where φ^k are the solutions corresponding to the constraint $\lambda = N-1$ we obtain the desired solutions. Of course, similar considerations, hold for the more general restricted Hartree equations corresponding to the functional (42) and we will skip them.

4) One possible way to avoid some of the difficulties encountered below in checking (P.S.-c^k) and thus solving the question mentioned in Remark 2) above would be to check and use a condition like

$$c^k < c^k(\lambda_1, \dots, \lambda_N) \quad \text{for all} \quad 0 \leqq \lambda_i \leqq 1 \quad \text{with} \quad \sum_{i=1}^N \lambda_i < N,$$

where $c^k(\lambda_1, \dots, \lambda_N)$ corresponds to the same inf-max value where the constraints defining M_{H} replaced by

$$\int_{\mathbb{R}^3} |\varphi_i|^2\,dx = \lambda_i \text{ for } 1 \leqq i \leqq N \left(\int_{\mathbb{R}^3} \varphi_i \varphi_j^*\,dx = \lambda_i \delta_{ij} \text{ for all } 1 \leqq i,j \leqq N \text{ for HF problems} \right).$$

Since we do not know how to check the above condition, we will not pursue this matter here.

5) Now, if we want to treat the H equations for $N \geqq 2$ without restricting a priori the form of the solutions or if we want to study the HF equations, there is another difficulty in addition to the spectral problem mentioned in Remark 2) above: even if this spectral difficulty is solved then for $N \geqq 2$ (P.S.-c) does not hold for all $c < 0$. Roughly speaking, this is due to the possible convergence of Palais-Smale sequences to points of the form $(\varphi_1, \dots, \varphi_p, 0, \dots, 0)$ for some $2 \leqq p < N$, where $(\varphi_1, \dots, \varphi_p)$ are solutions of the Hartree equations with N replaced by p. This may be rigorously justified as follows: let $2 \leqq p < N$, $(\varphi_1, \dots, \varphi_p)$ a solution for the Hartree equations with N replaced by p and $c = \mathscr{E}(\varphi_1, \dots, \varphi_p, 0, \dots, 0)$. Then we consider ψ^n in $\mathscr{D}(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} |\psi^n|^2\,dx = 1$, ψ^n converges to 0 in $L^p(\mathbb{R}^3)$ for $2 < p \leqq \infty$, $\nabla\psi^n$ converges to 0 in $L^q(\mathbb{R}^3)$ for $\frac{6}{5} < q \leqq \infty$, $D^2\psi^n$ converges to 0 in $L^r(\mathbb{R}^3)$ for $1 \leqq r \leqq \infty$. And our claim is proved since $\mathscr{E}(\varphi_1, \dots, \varphi_p, \psi^n, \dots, \psi^n) \underset{n}{\longrightarrow} 0$ and

$$(\mathscr{E}|_{M_{\mathrm{H}}})'(\varphi_1, \dots, \varphi_p, \psi^n, \dots, \psi^n) \underset{n}{\longrightarrow} 0 \quad \text{in} \quad (E^N)^*.$$

To avoid this loss of compactness at least when the spectral problem in Remark 2) above is solved, as it is the case in the spherically symmetric case, it is in a vague sense sufficient to show that

$$c^k < c_p^k \quad \text{for all} \quad 1 \leqq p < N,$$

where c_p^k corresponds to the same problem but with N replaced by p (and thus $c^k = c_N^k$) – observe that c_p^k corresponds to the choice $\lambda_1 = \dots = \lambda_p = 1$, $\lambda_{p+1} = \dots = \lambda_N = 0$ in $c^k(\lambda_1, \dots, \lambda_N)$ above. Again, we can solve this difficulty in the spherically symmetric situation. Indeed, let $p<N$, to each $(\varphi_1,\ldots,\varphi_p)\in H^1(\mathbb{R}^3)^p$ satisfying $\int_{\mathbb{R}^3}|\varphi_i|^2\,dx\leqq 1$, φ_i is radial for all i, we may associate in a continuous way the k first radial eigenfunctions of $\left[-\Delta+V+\varrho*\frac{1}{|x|}\right]$ – where $\varrho=\sum_{i=1}^{p}|\varphi_i|^2$ – that we denote by $\psi_1,\ldots,\psi_k\,\psi_1,\ldots,\psi_k$ are chosen such that

$$\psi_j(0)>0,\ \int_{\mathbb{R}^3}|\psi_j|^2\,dx=1\,.$$

Their existence is deduced from Lemma II.3 and the fact that $Z>N-1\geqq p$ and the continuous dependence comes from the fact that we are dealing with radial eigenfunctions (all radial eigenvalues are simple). Then for each $\xi\in S^{k-1}$, we have for all $\lambda\in\mathbb{R}$,

$$\mathscr{E}\left(\varphi_1,\ldots,\varphi_p,\lambda\sum_{i=1}^{k}\xi_i\psi_i\right)+\lambda^2\sum_{i=1}^{k}\xi_i^2\int_{\mathbb{R}^3}|\nabla\psi_i|^2+V|\psi_i|^2+\left(\varrho*\frac{1}{|x|}\right)|\psi_i|^2\,dx,$$

and using again Lemma II.3 this yields for all $R<\infty$,

$$\mathscr{E}\left(\varphi_1,\ldots,\varphi_p,\lambda\sum_{i=1}^{k}\xi_i\psi_i\right)\leqq\mathscr{E}(\varphi_1,\ldots,\varphi_p)-\lambda^2 v_R,\quad\text{for some}\quad v>0$$

for all $(\varphi_1,\ldots,\varphi_p)$ satisfying $\sum_{i=1}^{p}\int_{\mathbb{R}^3}|\varphi_i|^2\,dx\leqq p$. And this implies in a straightforward way $c_{p+1}^k<c_p^k$, $b_{p+1}^k<b_p^k\ldots$.

Again, to restrict the length of this paper and to avoid unpleasant technicalities, we will not make precise this matter here. □

Proof of Theorem III.2. We first prove that $c^k<0$. Exactly as in Sect. III.2 we can prove that for all $0<\lambda\leqq 1$,

$$c^k\leqq c^k(\lambda)=\operatorname*{Inf}_{h\in\Theta_\lambda^k}\ \operatorname*{Max}_{\xi\in S^{k-1}}\mathscr{E}(h(\xi)),$$

where Θ_λ^k is the collection of all continuous, odd mappings from S^{k-1} into

$$M_H^\lambda=\left\{\varphi\in H^1(\mathbb{R}^3)\Big/\int_{\mathbb{R}^3}|\varphi|^2\,dx=\lambda\right\}.$$

Hence, it is enough to prove that for λ small enough $c^k(\lambda)<0$. To this end we recall (see also Lemma III.1) that there exists a k-dimensional subspace V_k of $H^1(\mathbb{R}^3)$ such that

$$\forall\varphi\in V_k,\ \int_{\mathbb{R}^3}|\varphi|^2\,dx=1,\ \int_{\mathbb{R}^3}|\nabla\varphi|^2+V|\varphi|^2\,dx\leqq -v$$

for some $v>0$. The collection of those φ yields a sphere that we denote by S^{k-1} identifying ξ and φ. Then, we consider the mapping $h\in\Theta_\lambda^k$ defined by $h(\xi)=\sqrt{\lambda}\,\xi$. And we compute

$$\operatorname*{Max}_{\xi\in S^{k-1}}\mathscr{E}(h(\xi))\leqq -\lambda v+C\lambda^2;$$

obviously this is negative for $\lambda>0$ small enough.

Observe also that even if we take E, H as in (76), the above argument still yields the negativity of c^k.

Next, we show (74). Obviously enough the condition $\mathscr{E}(\varphi^k) < \mathscr{E}(0) = 0$ implies that φ^k is bounded in H^1 since $\varphi^k \in M_{\mathrm{H}}$. And as we have shown in the preceding sections the fact that $\varphi^k \xrightarrow[k]{} 0$ weakly in L^2 implies that

$$\int_{\mathbb{R}^3} |V|\varphi^k|^2\, dx \xrightarrow[k]{} 0,$$

therefore

$$\underline{\lim}_k\, \mathscr{E}(\varphi^k) = \underline{\lim}_k\, \mathscr{E}^\infty(\varphi^k) \geqq 0,$$

and (74) is proved.

To conclude, we just have to prove that (P.S.-c) holds for all $c < 0$. Indeed, if $(\varphi^n)_n \subset M_{\mathrm{H}}$ satisfies

$$(\mathscr{E}|_{M_{\mathrm{H}}})'(\varphi^n) \xrightarrow[n]{} 0 \quad \text{in} \quad (E)^*, \qquad \mathscr{E}(\varphi^n) \xrightarrow[n]{} c$$

we deduce that φ^n is bounded in E and thus

$$-\Delta\varphi^n + V\varphi^n + \left(|\varphi^n|^2 * \frac{1}{|x|}\right)\varphi^n + \varepsilon^n\varphi^n \xrightarrow[n]{} 0 \quad \text{in} \quad H_r^{-1},$$

where $\varepsilon^n = -\langle \mathscr{E}'(\varphi^n), \varphi^n \rangle$ is bounded in $\mathbb{R}$. Extracting enough subsequences if necessary we may assume that ε^n converges to some $\varepsilon \in \mathbb{R}$, φ^n converges weakly in $H^1(\mathbb{R}^3)$ to some $\varphi \in H_r^1$ as n goes to $+\infty$. Passing to the limit in n we obtain

$$-\Delta\varphi + V\varphi + \left(|\varphi|^2 * \frac{1}{|x|}\right)\varphi + \varepsilon\varphi = 0 \quad \text{in} \quad \mathbb{R}^3, \ \int_{\mathbb{R}^3} |\varphi|^2\, dx \leqq 1.$$

And, in addition, recalling that $\mathscr{E}$ is weakly lower semi-continuous we deduce that $\mathscr{E}(\varphi) \leqq c < 0$, hence $\varphi \not\equiv 0$.

Next, if $\int_{\mathbb{R}^3} |\varphi|^2\, dx = 1$, $\varphi^n \xrightarrow[n]{} \varphi$ in $L^2(\mathbb{R}^3)$ and from the equations we deduce

$$\begin{aligned}\overline{\lim}_n & \left\{\int_{\mathbb{R}^3} |\nabla\varphi^n|^2\, dx + D(|\varphi^n|^2, |\varphi^n|^2)\right\} \\ &= -\int_{\mathbb{R}^3} V|\varphi|^2 + \varepsilon|\varphi|^2\, dx = \int_{\mathbb{R}^3} |\nabla\varphi|^2\, dx + D(|\varphi|^2, |\varphi|^2),\end{aligned}$$

hence φ^n converges to φ in $H^1(\mathbb{R}^3)$ and (P.S.-c) is proved. Therefore we argue by contradiction and assume that $0 < \int_{\mathbb{R}^3} |\varphi|^2\, dx < 1$. In addition, we may assume that $\varepsilon \leqq 0$, since if $\varepsilon > 0$, we deduce again from the equations

$$\begin{aligned}\overline{\lim}_n & \left\{\int_{\mathbb{R}^3} |\nabla\varphi^n|^2 + \varepsilon|\varphi^n|^2\, dx + D(|\varphi^n|^2, |\varphi^n|^2)\right\} = -\int_{\mathbb{R}^3} V|\varphi|^2\, dx \\ &= \int_{\mathbb{R}^3} |\nabla\varphi|^2 + \varepsilon|\varphi|^2\, dx + D(|\varphi|^2, |\varphi|^2),\end{aligned}$$

and we reach a contradiction since this implies the convergence of φ^n to φ in $H^1(\mathbb{R}^3)$. And we conclude with the

Lemma III.1. *Let* $\varphi \in H^1(\mathbb{R}^3)$ *be a solution of*

$$-\Delta\varphi - \frac{Z}{|x|}\varphi + \left(\varrho * \frac{1}{|x|}\right)\varphi + \varepsilon\varphi = 0 \quad in \quad \mathbb{R}^3,$$

where $\varepsilon \leqq 0$, $\varrho \in L^1_+(\mathbb{R}^3)$, ϱ *is radial. Then, if* $Z > \int_{\mathbb{R}^3} \varrho\, dx$, $\varphi \equiv 0$.

Proof. We first rewrite $\left(\varrho * \frac{1}{|x|}\right)$ as $\int_{\mathbb{R}^3} \frac{\varrho(y)}{\max(|x|,|y|)}\, dy$ and we apply Theorem 3 of S. Agmon [1]: the conditions stated in [1] are verified as follows, let $p(x) = p_0(x) = \frac{Z}{|x|} - \varrho * \frac{1}{|x|} + |\varepsilon|$, then choosing α in $(0, \frac{1}{2})$, we compute

$$r^2\left(\frac{\partial p}{\partial r} + \frac{2(1-\alpha)}{r}p\right) \geqq (1-2\alpha)\left(Z - \int_{\mathbb{R}^3} \varrho\, dx\right) - 2(1-\alpha) \int_{|x| \geqq r} \varrho(x)\, dx$$
$$\geqq 0 \quad \text{for } r \text{ large enough.}$$

And thus by [1], we deduce that if $\varphi \not\equiv 0$

$$\varliminf_{R \to \infty} R^{-\alpha} \int_{1 \leqq |x| \leqq R} \frac{|\varphi(x)|^2}{|x|}\, dx > 0,$$

contradicting the fact that $\varphi \in L^2(\mathbb{R}^3)$. □

III.3. The Fixed Point Approach

We discuss in this section another approach to the existence of solutions of H, HF and related equations. This approach is, in some sense, the mathematical analogue of one numerical method often used by physicists to solve these equations. It was first studied mathematically by Wolkowisky [65] who proved the existence of solutions for (essentially) Hartree equations in the spherically symmetric case. However, our treatment of the existence of fixed points is somewhat different and probably simpler.

In order to illustrate the method, we start with HF equations and explain on this example the idea of the method. Then, we give and prove our main result. Finally, we conclude with a brief, non-exhaustive list of results which can be obtained for various equations by these arguments. We will define a mapping whose fixed points will yield solutions of HF equations (13). In fact, since we will have some spectral information on each φ_1, the mapping will depend on some set of integers: more precisely, let $n_1 < \ldots < n_N$ be N distinct integers. We may now define a mapping $T = T(n_1, \ldots, n_N)$ on a convex, closed subset of $L^2(\mathbb{R}^3 \times \mathbb{R}^3) \times L^1(\mathbb{R}^3)$: we first consider the set $\tilde{K} = \Big\{\varrho \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, $\tau \in L^1(\mathbb{R}^3)/\varrho \geqq 0$ a.e., $\tau \geqq 0$ a.e., $\int_{\mathbb{R}^3} \tau\, dx \leqq N$, $\varrho(x,y) = \varrho(y,x)$ a.e. and $\forall \varphi \in \mathcal{D}(\mathbb{R}^3)$, $0 \leqq \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \varrho(x,y)\varphi(x)\varphi(y)\, dx\, dy \leqq N \int_{\mathbb{R}^3} |\varphi(x)|^2 dx\Big\}$. Then, we consider the operator

$$-\Delta + V + \tau * \frac{1}{|x|} - \int_{\mathbb{R}^3} \varrho(x,y) \frac{1}{|x-y|} \cdot dy.$$

Observing that the self-adjoint operator given by

$$\psi \to \int_{\mathbb{R}^3} \varrho(x,y) \frac{1}{|x-y|} \psi(y)\, dy$$

is nonnegative, (indeed this is obvious if $\varrho(x,y) = \sum_{i=1}^{M} \psi_i(x)\psi_i(y)$ for some $M < \infty$, $\psi_i \in L^2 \quad \forall i$ and the general case follows), we deduce from Lemma II.3 that if $Z > N$ the above operator has infinitely many nagetive eigenvalues $(\lambda_k)_k \geqq 1$ (counted with their multiplicity). We then select the eigenvalues $\lambda_{n_1}, \dots, \lambda_{n_N}$ and consider the associated normalized eigenfunctions $\psi_1, \dots, \psi_N$. We then set

$$T(\varrho,\tau) = (\bar{\varrho},\bar{\tau}) \quad \text{where} \quad \bar{\varrho}(x,y) = \sum_{i=1}^{N} \psi_i(x)\psi_i(y), \quad \bar{\tau}(x) = \bar{\varrho}(x,x) = \sum_{i=1}^{N} |\psi_i(x)|^2. \tag{77}$$

Of course, only the last step is heuristic since in general eigenvalues may not be simple, in which case T is not properly defined. This is where we will be using the spherical symmetry (and it is the only place!): in general we do not know how to define T in a meaningful way or to avoid the possible multiplicities.

Hence, from now on, we will be dealing in this section only with the particular case when $V(x) = -\frac{Z}{|x|}$ and when all functions are radial (a better way of implementing spherical symmetry is described in the remarks below). More precisely, we denote by K the closed convex set of $L^2(\mathbb{R}^3 \times \mathbb{R}^3) \times L^1(\mathbb{R}^3)$ defined by

$$K = \Big\{ (\varrho,\tau) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3) \times L^1(\mathbb{R}^3) / \varrho \geqq 0 \text{ a.e.}, \ \tau \geqq 0 \text{ a.e.}, \ \varrho(x,y) = \varrho(y,x) \text{ a.e.},$$
$$\varrho(\mathcal{R}x, \mathcal{R}y) = \varrho(x,y), \ \tau(\mathcal{R}x) = \tau(x) \text{ a.e. for all rotations } \mathcal{R} \text{ of } \mathbb{R}^3, \ \int_{\mathbb{R}^3} \tau\, dx \leqq N,$$
$$0 \leqq \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \varrho(x,y)\varphi(x)\varphi(y)\, dx\, dy \leqq N \int_{\mathbb{R}^3} |\varphi|^2 dx \quad \text{for all} \quad \varphi \in \mathcal{D}(\mathbb{R}^3) \Big\},$$

and we now pick the simple eigenvalues $\lambda_{n_1} < \dots < \lambda_{n_N}$ of the operator $-\Delta + V + \left(\tau * \frac{1}{|x|}\right) - \int_{\mathbb{R}^3} \varrho(x,y) \frac{1}{|x-y|} \cdot dy$ acting on the space $L_r^2(\mathbb{R}^3) = \{ f \in L^2(\mathbb{R}^3) / f(\mathcal{R}x) = f(x)$ a.e. for all rotations $\mathcal{R}$ of $\mathbb{R}^3\}$. Let $\psi_{n_1}, \dots, \psi_{n_N}$ be the associated (radial) normalized eigenfunctions which exist by Lemma II.3 at least if $Z > N$: the ψ_j are well-defined (up to a change of sign), are orthogonal and thus $T(\varrho,\tau) = (\bar{\varrho},\bar{\tau})$ is still defined by (77). In view of Lemma II.3, the continuity of T is an easy exercise in functional analysis. If we show that T is compact on K, then by the Schauder theorem we obtain the following result.

Theorem III.3. *Assume $\bar{x}_j \equiv 0$ for all j,* i.e. $V = -\frac{Z}{|x|}$ *and $Z \geqq N$. Then for each set of integers $1 \leqq n_1 < n_2 < \dots < n_N$, there exists a solution $(\varphi_1, \dots, \varphi_N)$ in $H^1(\mathbb{R}^3)$*

of HF *equations* (14) *such that* $\int_{\mathbb{R}^3} \varphi_i \varphi_j dx = \delta_{ij}$ *for all* $1 \leqq i,j \leqq N$, $\varphi_1, \ldots, \varphi_N$ *are radial and for each i the Lagrange multiplier* ε_i *in* (14) *is nonnegative and is the opposite of the radial eigenvalue* λ_{n_i} *of the operator*

$$-\Delta + V + \varrho * \frac{1}{|x|} - \int \varrho(x,y) \frac{1}{|x-y|} \cdot dy$$

with $\varrho(x) = \varrho(x,x)$, $\varrho(x,y) = \sum_{i=1}^{N} \varphi_i(x) \varphi_i(y)$. *Furthermore, if* $Z > N$, *the eigenvalue* $(-\varepsilon_i)$ *is negative and* φ_i *decays exponentially fast at infinity for all* $1 \leqq i \leqq N$.

Remarks. 1) We prove in fact below that if $Z > N$, T is compact and thus we obtain the above result in the case $Z > N$. The case $Z = N$ is obtained by a limiting argument below.

2) There is a better notion of spherical symmetry than the one above (which corresponds to the real meaning of spherical symmetry in Physics). This notion may be easily explained on solutions of HF equations (14): assume that $(\varphi_1, \ldots, \varphi_N)$ is a solution of (14) such that $\varrho(\mathcal{R}x, \mathcal{R}y) = \varrho(x,y)$ for all rotations $\mathcal{R}$ of $\mathbb{R}^3$ (in particular ϱ is radial), then (take $Z > N$ to simplify) the eigenvalues of $\mathcal{H} = -\Delta + V + \varrho * \frac{1}{|x|} - R$, where $R\varphi = \int_{\mathbb{R}^3} \varrho(x,y) \frac{1}{|x-y|} \varphi(y)\, dy \quad (\forall \varphi \in \mathcal{D}(\mathbb{R}^3))$ may be classified as follows: let $\mu_k (k \geqq 1)$ be the eigenvalues of the Laplace-Beltrami operator on S^2, i.e. $\mu_k = k(k-1)$ with multiplicity $2k-1$, then for each $k \geqq 1$ consider the eigenvalues $\lambda_{n,k} (n \geqq 1)$ of $\mathcal{H} + \frac{\mu_k}{|x|^2}$ corresponding to radial eigenfunctions. Then, as it is standard, the collection $\{\lambda_{n,k}/n \geqq 1, k \geqq 1\}$ *is* the sequence of eigenvalues of $\mathcal{H}$. Hence, the Lagrange multipliers $\varepsilon_1, \ldots, \varepsilon_N$ are in that set and the consistency of spherical symmetry requires that if one of the ε_i corresponds to some $k \geqq 1$ then there are $(2k-2)$ indices distinct from i in $\{1, \ldots, N\}$ such that the corresponding ε_j are equal to ε_i and the associated ψ_i, ψ_j span precisely the eigenspace. In other words, instead of requiring in the definition of T all the φ_i to be radial and choosing the eigenvalues $\lambda_{n_1,1}, \ldots, \lambda_{n_N,1}$, we may choose $\lambda_{n_1,k_1}, \ldots, \lambda_{n_p,k_p}$ with $p \geqq 1$, $n_i \geqq 1$, $k_i \geqq 1$ for $1 \leqq i \leqq p$ and $n_i \neq n_j$ if $k_i = k_j$ for all $1 \leqq i \neq j \leqq p$, and where p, n_i, k_i are such that $\sum_{i=1}^{p} (2k_i - 1) = N$. Then, we define T as above, selecting the eigenfunctions as follows: for each k_i equal to 1 we take the normalized radial eigenfunctions and for each $k_i \geqq 2$ we take the $(2k_i - 1)$ normalized and orthogonal eigenfunctions spanning the eigenspace corresponding to λ_{n_i,k_i}. Then, we form $\varrho(x,y)$ with these N normalized and orthogonal eigenfunctions.

One checks easily that the above theorem still holds for such choices.

3) Let us recall that in the above result, φ_i has precisely $(n_i - 1)$ simple nodes. □

Proof of Theorem III.3. We first show that, if $Z > N$, T is compact, and then we consider the case $Z = N$. To prove the compactness of T, it is sufficient to show that $T(\varrho_m, \tau_m)$ is relatively compact in $L^2(\mathbb{R}^3 \times \mathbb{R}^3) \times L^1(\mathbb{R}^3)$ if $(\varrho_m, \tau_m) \in K$ is bounded in $L^2(\mathbb{R}^3\times\mathbb{R}^3)\times L^1(\mathbb{R}^3)$. Since $Z>N$, Lemma II.3 implies that eigenvalues $\lambda_{n_1}^m,\dots,\lambda_{n_N}^m$ and the corresponding eigenfunctions $\psi_1^m,\dots,\psi_n^m$ satisfy

$$(\psi_j^m)_m \quad \text{is bounded in} \quad H^1(\mathbb{R}^3) \quad \forall j,\ \ \lambda_{n_1}^m<\dots<\lambda_{n_N}^m\leqq -\varepsilon_0<0 \qquad \forall m\geqq 1$$

for some $\varepsilon_0>0$ independent of m. This implies obviously that $T(\varrho_m,\tau_m)$ is relatively compact in $L^2_{\mathrm{loc}}(\mathbb{R}^3\times\mathbb{R}^3)\times L^1_{\mathrm{loc}}(\mathbb{R}^3)$. Hence, we just have to check that

$$\int_{|x|\geqq R}|\psi_j^m|^2\,dx\to 0 \quad \text{as} \quad R\to\infty,\ \ \text{uniformly in } m \text{ for all } j.$$

If the exchange term (the operator K) were not present this would be almost obvious since ψ_j^m would be a normalized eigenfunction of $-\Delta+q-\lambda_{n_j}^m$, where q is radial and $q(r)\to 0$ as $r\to\infty$, and this would yield a uniform exponential decay of ψ_j^m using the fact that $\lambda_{n_j}^m\leqq -\varepsilon_0<0$.

Here, we may argue as follows: let $\chi\in C_b^\infty(\mathbb{R}^N)$, $\chi\equiv 0$ if $|x|\leqq\frac{1}{2}$, $\chi\equiv 1$ if $|x|\geqq 1$, $0\leqq\chi\leqq 1$ (we may choose χ radial if we wish). Then multiplying the equation satisfied by ψ_j^m by the quantity $\psi_j^m\chi_R^2$, where $\chi_R=\chi(\cdot/R)$ and integrating over $\mathbb{R}^3$, we deduce

$$\int_{\mathbb{R}^3}|\nabla\psi_j^m|^2\chi_R^2+\varepsilon_0|\psi_j^m|^2\chi_R^2\,dx\leqq\int_{\mathbb{R}^3}(-V)|\psi_j^m|^2\chi_R^2\,dx+2\int_{\mathbb{R}^3}\nabla\psi_j^m\nabla\chi_R\psi_j^m\chi_R\,dx$$
$$+\iint_{\mathbb{R}^3\times\mathbb{R}^3}\varrho^m(x,y)\frac{1}{|x-y|}\psi_j^m(x)\chi_R(x)\psi_j^m(y),$$

hence

$$\left(\varepsilon_0-\frac{2Z}{R}\right)\int_{\mathbb{R}^3}|\psi_j^m|^2\chi_R^2\,dx$$
$$\leqq\int_{\mathbb{R}^3}|\nabla\chi_R|^2|\psi_j^m|^2\,dx+C\left(\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{1}{|x-y|}|\psi_j^m|^2(x)\chi_R^2(x)|\psi_j^m(y)|^2\,dx\,dy\right)^{1/2}$$
$$\leqq\frac{C}{R^2}+C\left(\iint_{\mathbb{R}^3\times\mathbb{R}^3}|\psi_j^m(x)|^2\chi_R^2(x)\frac{1}{\max(|x|,|y|)}|\psi_j^m(y)|^2\,dx\,dy\right)^{1/2},$$
$$\leqq\frac{C}{R^2}+\frac{C}{\sqrt{R}},$$

where C denotes various constants independent of m, and we conclude.

Having thus proved the existence of solutions for $Z>N$, we now treat the case when $Z=N$. In that case, we approximate Z by $Z+\varepsilon$, find by the above proof a solution $(\varphi_1^\varepsilon,\dots,\varphi_N^\varepsilon)$ of HF equations (14) satisfying all the conditions stated in the theorem. We denote, with obvious notations, by $\mathscr{H}_\varepsilon$ the operator $-\Delta-\frac{Z+\varepsilon}{|x|}+\varrho^\varepsilon*\frac{1}{|x|}-\int\varrho^\varepsilon(x,y)\frac{1}{|x-y|}\cdot dy$ and by $\lambda_{n_1}<\dots<\lambda_{n_N}$ the eigenvalues of $\mathscr{H}_\varepsilon$ (of order $n_1,\dots,n_N$). The functions $(\varphi_1^\varepsilon,\dots,\varphi_N^\varepsilon)$ are clearly bounded in $H^1(\mathbb{R}^3)$ (bounded in L^2 by definitions and the gradient bound is deduced from the equation) and, extracting if necessary subsequences, we may assume that $\varphi_i^\varepsilon\underset{\varepsilon}{\longrightarrow}\varphi_i$ weakly in $H^1(\mathbb{R}^3)$. If $\int_{\mathbb{R}^3}\varrho\,dx=\sum_{i=1}^N\int_{\mathbb{R}^3}|\varphi_i|^2\,dx<N$ then the limit operator

$\mathscr{H}$ admits infinitely many negative eigenvalues (use again Lemma II.3): in particular, $\lambda_{n_1} < \ldots < \lambda_{n_N} < 0$ and $\lambda^\varepsilon_{n_i} \underset{\varepsilon}{\longrightarrow} \lambda_{n_i}$. But this means that there exists $\varepsilon_0 > 0$ such that for ε small enough

$$\lambda^\varepsilon_{n_1} < \ldots < \lambda^\varepsilon_{n_N} \leqq -\varepsilon_0 < 0 .$$

Then, the proof above applies and we deduce the strong convergence of φ^ε to φ_i in $L^2(\mathbb{R})$ reaching a contradiction. Therefore, $\int_{\mathbb{R}^3} \varrho\, dx = N$ and $\varphi^\varepsilon_i \underset{\varepsilon}{\longrightarrow} \varphi_i$ in $L^2(\mathbb{R}^3)$ for $1 \leqq i \leqq N$. The strong convergence in $H^1(\mathbb{R}^3)$ is deduced from the equations as usual and the rest of Theorem III.3 follows. □

We now conclude this section with two applications of the above method: the first one is a slightly more general form of the restricted Hartree equations [Euler-Lagrange equations associated with (42)–(43)] and the second one is the equation associated with (47)–(48) containing in particular the TFW and the TFDW equations. Hence, the first set of equations we will consider is

$$-\Delta\varphi_i + V_i(r)\,\varphi_i + \sum_{j=1}^{N} a_{ij}\left(|\varphi_j|^2 * \frac{1}{|x|}\right)\varphi_i + \varepsilon_i\,\varphi_i = 0 \quad \text{in} \quad \mathbb{R}^3,$$
$$\text{for all} \quad 1 \leqq i \leqq N \tag{78}$$

with the constraints $\int_{\mathbb{R}^3} |\varphi_i|^2\, dx = \lambda_i$, where $\lambda_i > 0$, $a_{ij} \geqq 0$ and $a_{ij} = a_{ji}$ for all i, j, and for all i, $V_i(r)$ satisfies

$$\exists \varepsilon_0 \in (0, \tfrac{1}{4}), \qquad \left(V_i + \frac{\varepsilon_0}{r^2}\right)^- \in L^\infty(\mathbb{R}^3) + L^{3/2}(\mathbb{R}^3)$$
$$\forall \varepsilon > 0, \qquad \left(V_i + \frac{Z-\varepsilon}{r}\right)^+ \in L^1(\mathbb{R}^3) + L^3(\mathbb{R}^3). \tag{79}$$

For instance, $V_i(r) = -\dfrac{Z}{r} + \dfrac{a_i}{r^2}$ satisfies (79) if $a_i > -\frac{1}{4}$.

Then, if $n_1 < n_2 < \ldots < n_N$ are N fixed distinct integers, we define a mapping $T(\varrho_1, \ldots, \varrho_N)$ defined on the convex set

$$K = \left\{(\varrho_1, \ldots, \varrho_N) \in L^1(\mathbb{R}^3)^N / 0 \leqq \varrho_i, \ \text{pi is radial}, \ \int_{\mathbb{R}^3} \varrho_i\, dx \leqq \lambda_i \quad \text{for all} \quad i\right\}$$

by $(\bar\varrho_1, \ldots, \bar\varrho_N)$, where $\bar\varrho_i = |\varphi_i|^2$ and φ_i is the radial normalized eigenfunction of the operator $h_i = -\Delta + V_i + \sum_{j=1}^{N} a_{ij}\left(\varrho_j * \dfrac{1}{|x|}\right)$ corresponding to the n_i eigenvalue. This is possible by Lemma II.3 and (79) if $Z > \sum_j a_{ij}\lambda_j$ for all i and again by a limiting procedure we prove as above the

Theorem III.4. *We assume* (79) *and for each i either* $\sum_j a_{ij}\lambda_j < Z$, *or* $\sum_j a_{ij}\lambda_j = Z$, *and there exists j such that* $\sum_k a_{jk}\lambda_k = Z$, $a_{ij} > 0$. *Then, for each set of integers* $1 \leqq n_1 < n_2 < \ldots < n_N$, *there exists a solution* $(\varphi_1, \ldots, \varphi_N)$ *in* $H^1(\mathbb{R}^3)^N$ *of* (78) *such that* $\int_{\mathbb{R}^3} |\varphi_i|^2\, dx = \lambda_i$ *for all i*, $\varphi_1, \ldots, \varphi_N$ *are radial and for all i the Lagrange* *multiplier* ε_i *in* (78) *is nonnegative and is the opposite of the radial eigenvalue* λ_{n_i} *of the operator*

$$-\Delta + V_i + \sum_{j=1}^{N} a_{ij}\left(|\varphi_j|^2 * \frac{1}{|x|}\right).$$

Furthermore, if $Z > \sum_j a_{ij}\lambda_j$, $\varepsilon_i > 0$ *and* φ_i *decays exponentially at infinity.*

Remark. This result contains Wolkowisky's result [65] which corresponds to the case $V_i(r) = -\frac{Z}{r} + \frac{a_i}{r^2}$ for some $a_i > 0$, $a_{ij} = 1 - \delta_{ij}$, $\lambda_i = 1$, $Z > (N-1)$.

We conclude with the equation

$$-\Delta\varphi - \frac{Z}{|x|}\varphi + \left(|\varphi|^2 * \frac{1}{|x|}\right)\varphi + \frac{1}{2}f(\varphi) + \varepsilon\varphi = 0 \quad \text{in } \mathbb{R}^3 \tag{80}$$

with the constraint $\int_{\mathbb{R}^3} |\varphi|^2 dx = \lambda$, where $\lambda > 0$ and f is an odd C^1 function on $\mathbb{R}$ such that $f(0) = f'(0) = 0$ and

$$|f(t)| = o(|t|^{7/3}) \quad \text{as } t \to \infty, \quad f^+(t) = 0(t^{5/3}) \quad \text{as } t \to 0_+ \tag{81}$$

(the analogue of (58)–(49)). Notice that (80) is the Euler-Lagrange equation associated with the minimization problem (47)–(48). For

$$\varrho \in K = \left\{ z \in L^1(\mathbb{R}^3)/z \geqq 0, \quad z \text{ is radial } \int_{\mathbb{R}^3} z\,dx \leqq \lambda \right\}$$

we define a mapping T by $Tz = |\varphi|^2$, where φ is the radial normalized eigenfunction corresponding to the eigenvalue λ_k (for some fixed integer $k \geqq 1$) of

$$-\Delta - \frac{Z}{r} + \left(\varrho * \frac{1}{|x|}\right) + \frac{1}{2}f(\varrho^{1/2})\,\varrho^{-1/2}.$$

We claim that Lemma II.3 implies that such an eigenfunction exists if $Z > \lambda$. Indeed, denoting by $q = \frac{1}{2}f(\varrho^{1/2})\,\varrho^{-1/2}$, we deduce from (81) first of all that

$$q \geqq -C_\varepsilon - \varepsilon\varrho^{2/3},$$

hence the operator is bounded from below on the sphere of L^2, and next that

$$q^+ \leqq C(\varrho^{1/3} + \varrho^{2/3}) \in L^3 + L^{3/2},$$

and Lemma II.3 applies. And we obtain the

Theorem III.5. *Assume* (81) *and* $Z \geqq \lambda$. *Let* $k \geqq 1$, *then there exists a radial solution in* $H^1(\mathbb{R}^3)$ *of* (80) *such that* $\int_{\mathbb{R}^3} |\varphi|^2 dx = \lambda$ *and the Lagrange multiplier* ε *is nonnegative and is the opposite of the radial eigenvalue* λ_k *of the operator*

$$-\Delta - \frac{Z}{r} + |\varphi|^2 * \frac{1}{|x|} + \frac{1}{2}f(\varphi)\,\varphi^{-1}.$$

Furthermore, if $Z > \lambda$, $\varepsilon > 0$ *and* φ *decays exponentially at infinity.*

Proof. Again, the case $Z=\lambda$ is obtained by a limiting procedure. If $Z<\lambda$, we just have to check that T is compact on K and this is done exactly as in the proof of Theorem III.3. □

IV. General Existence Results

The organization of this section is the following: we first state our main existence results for H and HF equations and we briefly explain the strategy of proof in Sect. IV.1. The actual proof is given in Sect. IV.2, and we explain in Sect. IV.3 how this method also yields various existence results for related equations.

IV.1. Main Results and Presentation of the Method

Of course, when dealing with H equations (respectively HF equations), the functional $\mathscr{E}$ will be the one given by (7) [respectively (9)]. With this convention our main result is the

Theorem IV.1.

1) H *equations: Assume* $Z>(N-1)$. *There exists a sequence* $((\varphi_1^k, \ldots, \varphi_N^k))_{k\geq 1}$ *of distinct solutions of Hartree equations* (11) *in* $H^1(\mathbb{R}^3)^N$ *which satisfy:* $\int_{\mathbb{R}^3} |\varphi_i^k|^2\,dx=1$, $\forall\, 1\leqq i\leqq N$, $\forall\, k\geqq 1$. *In addition, the Lagrange multipliers* $(-\varepsilon_i^k)$ *are positive and* φ_i^k *decays exponentially at infinity for all* i, k. *Finally, as* k *goes to* ∞, $\varepsilon_i^k \xrightarrow[k]{} 0$,

$$\nabla\varphi_i^k \xrightarrow[k]{} 0 \quad \text{in} \quad L^2(\mathbb{R}^3), \quad \varphi_i^k \xrightarrow[k]{} 0 \quad \text{in} \quad L^p(\mathbb{R}^3) \quad \text{for} \quad 2<p\leqq\infty\,.$$

2) HF *equations: Assume* $Z\geqq N$. *There exists a sequence* $((\varphi_1^k, \ldots, \varphi_N^k))_{k\geq 1}$ *of distinct solutions of Hartree-Fock equations* (13) *in* $H^1(\mathbb{R}^3)^N$ *which satisfy:* $\int_{\mathbb{R}^3} \varphi_i^k \varphi_j^{k*}\,dx=\delta_{ij}$ *for all* $1\leqq i,j\leqq N$, $k\geqq 1$. *In addition, the Lagrange multipliers* $(-\varepsilon_i^k)$ *are nonnegative and if* $Z>N$, *they are positive and the functions* φ_i^k *decay exponentially at infinity for all* i, k. *Finally, as* k *goes to* ∞,

$$\varepsilon_i^k \xrightarrow[k]{} 0, \quad \nabla\varphi_i^k \xrightarrow[k]{} 0 \quad \text{in} \quad L^2(\mathbb{R}^3), \quad \varphi_i^k \xrightarrow[k]{} 0 \quad \text{in} \quad L^p(\mathbb{R}^3) \quad \text{for} \quad 2<p\leqq\infty. \quad \square$$

We next sketch the proof of the above theorem. To this end, we need a few notations. We will approximate the H or HF equations by similar equations the only difference being that we replace $\mathbb{R}^3$ by a ball B_R and we will let $R\to\infty$. We will always consider $H_0^1(B_R)$ as a closed subspace of $H^1(\mathbb{R}^3)$ extending functions in $H_0^1(B_R)$ by 0 outside B_R. In the *first step*, we consider the values c_R^k which are defined by (71), where we choose $H=L^2(B_R)$, $E=H_0^1(B_R)$, and $\mathscr{E}$ is the functional corresponding to H or HF equations. We check that for each $k\geqq 1$, $c_R^k \downarrow c^k$ as $R\uparrow +\infty$, where c^k corresponds to the same value where $H=L^2(\mathbb{R}^3)$, $E=H^1(\mathbb{R}^3)$ and we recall that $c^k<0$, $c^k\uparrow 0$ as $k\uparrow\infty$.

In the *second step*, we deduce from the results of A. Bahri [4] that if k is chosen such that $c_k<c_{k+1}$, then for R large enough there exists a critical point $(\varphi_1^R, \ldots, \varphi_N^R)$ of $\mathscr{E}|_{M_{\mathrm{H}}}$ or $\mathscr{E}|_{M_{\mathrm{HF}}}$ in $H_0^1(B_R)^N$ such that

$$c_k^R \leqq \mathscr{E}(\varphi_1^R, \ldots, \varphi_N^R)\leqq M_k \quad \text{for some constant } M_k \text{ ind. of } R, \tag{82}$$

and the number of negative eigenvalues of the quadratic form defined by

$$\mathscr{E}''(\varphi^R) - \langle \mathscr{E}'(\varphi^R), \varphi^R \rangle, \quad \text{with} \quad \varphi^R = (\varphi_1^R, \ldots, \varphi_N^R)$$

is bounded from above by k.

Finally, in the *third step* we show that φ^R converges in $H^1(\mathbb{R}^3)^N$ to some solution φ of H or HF equations (this is where we use the assumption on Z) which satisfies $c_k \leqq \mathscr{E}(\varphi) < 0$, where k is still chosen as above. This enables us to conclude the proof of Theorem IV.1.

We would like to mention that the convergence argument in step 3 is the same as the ones introduced in Sect. II, and that step 1 is very easy. Let us also remark that we could also have used the critical points results due to Viterbo [64] or Coffman [21], modifying a bit the above scheme of proof but keeping the same basic ingredient namely a bound on the Morse index of some convenient critical point.

To conclude this section, we wish to point out how the above arguments fail if $N-1 < Z < N$ for HF equations. Indeed, in this case, we only build a sequence $((\varphi_1^k, \ldots, \varphi_N^k))_{k \geqq 1}$ of solutions of HF equations (13) in $H^1(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} \varphi_i^k \varphi_j^k \, dx = 0$ if $i \neq j$ and for each $k \geqq 1$

$$\text{either} \qquad \int_{\mathbb{R}^3} (\varphi_i^k)^2 \, dx = 1 \qquad \text{for all } i,$$

$$\text{or} \qquad Z \leqq \sum_{i=1}^{N} \int_{\mathbb{R}^3} (\varphi_i^k)^2 \, dx < N \qquad \text{and for each } i$$

$$\int_{\mathbb{R}^3} (\varphi_i^k)^2 \, dx < 1 \qquad \text{implies} \qquad \varepsilon_i^k = 0 .$$

In the case of minima this alternative was sufficient to conclude (by excluding the second possibility) but for more general critical points we were not able to get around this difficulty. From the Physics viewpoint however, there is no difference between the assumptions $Z > N-1$ or $Z \geqq N$ since Z is integer-valued!

IV.2. Proofs

Step 1. By the very definition of c_k^R we see that $c_k^R \downarrow$ as $R \uparrow \infty$ and that $c_k^R \geqq c_k$ for all $R < \infty$. In addition, we already know from Theorem III.2 that $c_k < 0$ and that $c_k \uparrow 0$ as $k \uparrow \infty$.

To conclude, we just have to show that $c_k = \lim_{R \uparrow \infty} c_k^R$. To this end let $\varepsilon > 0$ and let $h \in \Theta^k$ [i.e. an odd continuous map from S^{k-1} into M_{H} or M_{HF}, with the choice of spaces $E = H^1(\mathbb{R}^3)$, $H = L^2(\mathbb{R}^3)$] be such that

$$c_k \leqq \operatorname*{Max}_{\xi \in S^{k-1}} \mathscr{E}(h(\xi)) \leqq c_k + \varepsilon .$$

Then, we observe that $h(S^{k-1})$ is a compact set in $H^1(\mathbb{R}^3)$ and we wish to deduce from this fact an approximated map h_R still odd and continuous from S^{k-1} into the manifolds M_{H} or M_{HF} corresponding now to the choices of spaces $E = H_0^1(B_R)$, $H = L^2(B_R)$ and such that

$$\operatorname*{Max}_{\xi \in S^{k-1}} \| h(\xi) - h_R(\xi) \|_{H^1(\mathbb{R}^3)} \to 0 \quad \text{as} \quad R \to \infty . \tag{83}$$

If this is the case, we conclude since we deduce

$$c_k^R \leqq \underset{\xi \in S^{k-1}}{\operatorname{Max}} \mathscr{E}(h_R(\xi)) \leqq \underset{\xi \in S^{k-1}}{\operatorname{Max}} \mathscr{E}(h(\xi)) + \delta_R \leqq c_k + \varepsilon + \delta_R,$$

where $\delta_R \to 0$ as $R \to \infty$.

Next, to prove (83) we first truncate the functions given by $h(S^{k-1})$, i.e. we consider $\chi \in \mathscr{D}(\mathbb{R}^3)$, $0 \leqq \chi \leqq 1$, $\chi \equiv 1$ on $B_{1/2}$, $\chi \equiv 0$ if $|x| \geqq 1$, and we set $\chi_R(x) = \chi\left(\frac{x}{R}\right)$; then we denote by

$$\tilde{h}_R(\xi) = (\chi_R h_1(\xi), \ldots, \chi_R h_N(\xi)), \quad \forall \xi \in S^{k-1},$$

where h_i denote obviously the components of the map h. Using the compactness of $h(\xi)$ it is straightforward to deduce

$$\underset{\xi \in S^{k-1}}{\operatorname{Max}} \| h(\xi) - \tilde{h}_R(\xi) \|_{H^1(\mathbb{R}^3)} \to 0 \quad \text{as} \quad R \to \infty.$$

In the case of H problems, we conclude by setting for R large enough (so that $\underset{\xi \in S^{k-1}}{\operatorname{Min}} \| \tilde{h}_{R,i}(\xi) \|_{L^2(B_R)} > 0$)

$$h_R(\xi) = (\tilde{h}_{R,i}(\xi) \| \tilde{h}_{R,i}(\xi) \|_{L^2(B_R)}^{-1})_{1 \leqq i \leqq N}.$$

In the case of HF problems, we build the map h_R for R large enough by a standard orthonormalization procedure

$$h_{R,1}(\xi) = \tilde{h}_{R,1}(\xi) \| \tilde{h}_{R,1}(\xi) \|_{L^2(B_R)}^{-1},$$

and for $2 \leqq i \leqq N$,

$$h_{R,i}(\xi) = \left\{ \tilde{h}_{R,i}(\xi) - \sum_{j=1}^{i-1} (\tilde{h}_{R,i}(\xi), h_{R,j}(\xi))_{L^2} h_{R,j}(\xi) \right\} \cdot$$

$$\cdot \left\| \tilde{h}_{R,i}(\xi) - \sum_{j=1}^{i-1} (\tilde{h}_{R,i}(\xi), h_{R,j}(\xi))_{L^2} h_{R,j}(\xi) \right\|_{L^2(B_R)}^{-1},$$

and we conclude observing that h_R is still odd and continuous.

Step 2. We choose $k \geqq 1$ such that $c_k < c_{k+1}$. In view of the results proved in step 1, we still have $c_k^R < c_{k+1} \leqq c_{k+1}^R$ for R large enough say $R \geqq R_0 \geqq 1$. Then, choosing $R = R_0$, there exists $h_0 \in \Theta_k^{R_0}$ (odd continuous map from S^{k-1} into the manifold $M_H^{R_0}$ or $M_{\mathrm{HF}}^{R_0}$ corresponding to $H_0^1(B_{R_0})$, $L^2(B_{R_0})$ such that

$$\underset{\xi \in S^{k-1}}{\operatorname{Max}} \mathscr{E}(h_0(\xi)) < c_{k+1}.$$

We then chose $\bar{e} \in H_0^1(B_{R_0})^N$ such that

$$\int_{B_{R_0}} \bar{e}_i \bar{e}_j \, dx = \delta_{ij}, \quad \int_{B_{R_0}} \bar{e}_i h_{0,j}(\xi) \, dx = 0 \quad \forall \xi \in S^{k-1}, \quad \forall 1 \leqq i,j \leqq N,$$

and we consider the set

$$A = \{t^{1/2} h(\xi) + (1-t)^{1/2} \bar{e} / t \in [0,1], \xi \in S^{k-1}\} \subset M_{\mathrm{HF}}$$

(with a similar construction if we are in the case of H problems). Then, we denote by $M_k = \sup\{\mathscr{E}(u)/u \in A\}$.

We now deduce from the results and methods of Bahri [4] that there exists for each $R \geqq R_0$ [notice that $\Theta_k^R \supset \Theta_k^{R_0}$, since $H_0^1(B_R) \supset H_0^1(B_{R_0})$] a critical point $(\varphi_1^R, \dots, \varphi_N^R)$ of $\overline{\mathscr{E}}^R$ (the restriction of $\mathscr{E}$ to M_{H}^R or M_{HF}^R) and thus in $H_0^1(B_R)^N$ such that

$$c_k^R \leqq \mathscr{E}(\varphi_1^R, \dots, \varphi_N^R) \leqq M_k,$$

and the number of negative eigenvalues (counted with their multiplicities) of the quadratic form $\mathscr{E}''(\varphi^R) - \langle \mathscr{E}'(\varphi^R), \varphi^R\rangle$ is bounded from above by k. In other words, taking for example the case of HF problems with real-valued functions to simplify notations, $(\varphi_1^R, \dots, \varphi_N^R) \in H_0^1(B_R)^N$ and satisfy

$$-\Delta\varphi_i^R + V\varphi_i^R + \left(\varrho^R * \frac{1}{|x|}\right)\varphi_i^R - \int \varrho^R(x,y)\frac{1}{|x-y|}\varphi_i^R(y)\,dy + \varepsilon_i^R\varphi_i^R = 0 \quad \text{in } B_R \tag{84}$$

$$\int \varphi_i^R \varphi_j^R\,dx = \delta_{ij} \quad \text{for } 1 \leqq i,j \leqq N \tag{85}$$

$$\begin{aligned}&\sum_{i=1}^N \int |\nabla\psi_i|^2 + V|\psi_i|^2 + \left(\varrho^R * \frac{1}{|x|}\right)|\psi_i|^2 + \varepsilon_i^R|\psi_i|^2\,dx \\ &- \sum_{i=1}^N \iint \varrho^R(x,y)\frac{1}{|x-y|}\psi_i(x)\psi_i(y)\,dx\,dy \\ &+ 2\sum_{i,j=1}^N \iint \varphi_i^R(x)\psi_i(x)\frac{1}{|x-y|}\varphi_j^R(y)\psi_j(y) \\ &- \varphi_i^R(x)\psi_i(y)\frac{1}{|x-y|}\varphi_j^R(x)\psi_j(y)\,dx\,dy \geqq 0\end{aligned} \tag{86}$$

for all $(\psi_1, \dots, \psi_N)$ in a closed subspace of $H_0^1(B_R)^N$ of codimension at most $k+N$, where $\varrho^R(x) = \sum_{i=1}^N |\varphi_i^R(x)|^2$, $\varrho^R(x,y) = \sum_{i=1}^N \varphi_i^R(x)\varphi_i^R(y)$ and $\varepsilon_i^R = -\left\langle \frac{\partial\mathscr{E}}{\partial\varphi_i}(\varphi_1^R, \dots, \varphi_N^R), \varphi_i^R\right\rangle$.

Step 3. We first show that φ^R converges in $H^1(\mathbb{R}^3)^N$ to some solution of H or HF equations. Combining (82) and (85) we see that φ^R is bounded in $H^1(\mathbb{R}^3)^N$ and thus ε_i^R are bounded. Then, in view of arguments we did several times in the preceding sections it is enough to show that $\varliminf_{R\to\infty} \varepsilon_i^R > 0$ (at least if $Z > N$ in HF problems, the case $Z = N$ being treated by the same modifications as the ones we did several times before). And this is achieved exactly as in the preceding sections by the combined use of Lemma II.2, Lemma II.3 and (86).

Hence, we obtain a solution φ (depending on the integer k we chose at the beginning of Sect. II) of H or HF equations which satisfies in addition

$$\int_{\mathbb{R}^3} |\varphi_i|^2\,dx = 1, \quad \varepsilon_i > 0 \quad \text{for all } 1 \leqq i \leqq N, \quad \text{in the H case} \tag{87}$$

$$\int_{\mathbb{R}^3} \varphi_i\varphi_j^*\,dx = \delta_{ij}, \quad \varepsilon_i \geqq 0 \quad \text{for all } 1 \leqq i,j \leqq N, \quad \varepsilon_i > 0 \tag{88}$$

for all $1 \leqq i \leqq N$ if $Z > N$, in the HF case.

We next observe that $c_k \leqq \mathscr{E}(\varphi_1, \dots, \varphi_N)$ and

$$0 \geqq -\sum_{i=1}^{N} \varepsilon_i = \sum_{i=1}^{N} \int_{\mathbb{R}^3} |\nabla \varphi_i|^2 + V|\varphi_i|^2 \, dx$$

$$+ \sum_{i \neq j} D(|\varphi_i|^2, |\varphi_j|^2) > \mathscr{E}(\varphi_1, \dots, \varphi_N) \quad \text{in the H case,}$$

while in the HF case

$$0 \geqq -\sum_{i=1}^{N} \varepsilon_i = \sum_{i=1}^{N} \int_{\mathbb{R}^3} |\nabla \varphi_i|^2 + V|\varphi_i|^2 \, dx$$

$$+ \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \{\varrho(x)\varrho(y) - \varrho(x,y)^2\} \frac{1}{|x-y|} \, dx\, dy > \mathscr{E}(\varphi_1, \dots, \varphi_N),$$

since $\varrho(x)\varrho(y) - \varrho(x,y)^2 \geqq 0$, $\not\equiv 0$ on $\mathbb{R}^3 \times \mathbb{R}^3$.

To obtain the existence of a sequence of distinct solutions we just observe that once we have built m distinct solutions satisfying

$$c_{k_l} \leqq \mathscr{E}(\varphi_1^l, \dots, \varphi_N^l) < c_{k_{l+1}} \leqq \mathscr{E}(\varphi_1^{l+1}, \dots, \varphi_N^{l+1}) < 0$$

for $1 \leqq l \leqq m$, where $k_1 < \dots < k_m$ are m integers, then we choose an integer $k > k_m$ such that

$$\mathscr{E}(\varphi_1^m, \dots, \varphi_N^m) < c_k < c_{k+1}.$$

This is possible since $c_k \uparrow 0$ as $k \uparrow \infty$ and $\mathscr{E}(\varphi_1^m, \dots, \varphi_N^m) < 0$. Then, we obtain by the arguments above a solution $(\varphi_1^{m+1}, \dots, \varphi_N^{m+1})$ satisfying

$$c_k \leqq \mathscr{E}(\varphi_1^{m+1}, \dots, \varphi_N^{m+1}) < 0,$$

and we build the desired sequence setting $k = k_{m+1}$. Observe also that the sequence of solutions we built satisfies (87), (88) for all $k \geqq 1$ and

$$\mathscr{E}(\varphi_1^k, \dots, \varphi_N^k) \uparrow 0 \quad \text{as} \quad k \uparrow \infty.$$

And by the argument used above to show the negativity of $\mathscr{E}(\varphi_1, \dots, \varphi_N)$ we deduce

$$\sum_{i \neq j} D(|\varphi_i^k|^2, |\varphi_j^k|^2) \xrightarrow[k]{} 0 \quad \text{in the H case,} \tag{89}$$

$$\iint_{\mathbb{R}^3 \times \mathbb{R}^3} \{\varrho^k(x)\varrho^k(y) - \varrho^k(x,y)^2\} \frac{1}{|x-y|} \, dx\, dy \xrightarrow[k]{} 0 \text{ in the HF case.} \tag{90}$$

On the other hand (87) and $\mathscr{E}(\varphi_1^k, \dots, \varphi_N^k) < 0$ imply that φ_i^k is bounded in $H^1(\mathbb{R}^3)$. And this combined with (89)–(90) yields easily that

$$\varphi_i^k \xrightarrow[k]{} 0 \quad \text{weakly in } H^1(\mathbb{R}^3) \quad \text{for all} \quad 1 \leqq i \leqq N.$$

Observe also that $\varepsilon_i^k \xrightarrow[k]{} 0$ for all $1 \leqq i \leqq N$. And then from the H or HF equations one deduces easily that $\nabla \varphi_i^k \xrightarrow[k]{} 0$ in $L^2(\mathbb{R}^3)$, and we may conclude.

IV.3. Related Equations

Using exactly the same method, we obtain the results presented below; hence, we will only state them.

We begin with a general form of the restricted Hartree equations,

$$-\Delta\varphi_i + V_i(x)\varphi_i + \sum_{j=1}^{N} a_{ij}\left(|\varphi_j|^2 * \frac{1}{|x|}\right)\varphi_i + \varepsilon_i\varphi_i = 0 \quad \text{in} \quad \mathbb{R}^3,$$
$$\text{for all} \quad 1 \leqq i \leqq N, \tag{91}$$

with the constraints $\int_{\mathbb{R}^3} |\varphi_i|^2\,dx = \lambda_i$ for all $1 \leqq i \leqq N$, where $a_{ij} = a_{ji} \geqq 0$, $\lambda_i > 0$ and V_i satisfies (79). Our main existence result is the

Theorem IV.2. *Assume that for all* $1 \leqq i \leqq N$, $Z > \sum_{j=1}^{N} a_{ij}\lambda_j$ *or* $Z = \sum_{j=1}^{N} a_{ij}\lambda_j$, *and there exists k such that* $Z = \sum_{j=1}^{N} a_{jk}\lambda_j$ *and* $a_{ik} > 0$. *Assume also that the potentials* V_i *satisfy* (79) *for all* $1 \leqq i \leqq N$. *Then, there exists a sequence* $((\varphi_1^k, \dots, \varphi_N^k))_{k \geqq 1}$ *of distinct solutions of* (91) *in* $H^1(\mathbb{R}^3)$ *which satisfy* $\int_{\mathbb{R}^3} |\varphi_i^k|^2\,dx = \lambda_i$ *for all* $1 \leqq i \leqq N$, $k \geqq 1$. *In addition, the multiplier* ε_i^k *is nonnegative and if for some i* $Z > \sum_{j=1}^{N} a_{ij}\lambda_j$, *then* $\varepsilon_i^k > 0$ *for all* $k \geqq 1$; *in that case* φ_i^k *decays exponentially at infinity for all* $k \geqq 1$. *Finally,* $\varepsilon_i^k \xrightarrow[k]{} 0$, $\varphi_i^k \xrightarrow[k]{} 0$ *in* $L^p(\mathbb{R}^3)$ *for* $2 < p \leqq \infty$, $\nabla\varphi_i^k \xrightarrow[k]{} 0$ *in* $L^2(\mathbb{R}^3)$ *for all* $1 \leqq i \leqq N$. □

And we conclude with an extended form of TFW type equations: by this example, we wish to show how one can extend our results and methods for problems in $\mathbb{R}^N$ with more general potentials V, or interactions different from $\frac{1}{|x|}$.... We consider the equation

$$-\Delta\varphi + V\varphi + (|\varphi|^2 * W) + f(\varphi) + \varepsilon\varphi = 0 \quad \text{in} \quad \mathbb{R}^N, \tag{92}$$

with the constraint $\int_{\mathbb{R}^3} |\varphi|^2\,dx = \lambda$, where $\lambda > 0$, $N \geqq 3$ and V, W satisfy (for instance)

$$V^- \in L^{N/2}(\mathbb{R}^N) + L^p(\mathbb{R}^N) \quad \text{for some} \quad \frac{N}{2} < p < \infty$$
$$\forall \varepsilon > 0, \left(V + \frac{Z-\varepsilon}{|x|^\alpha}\right)^+ \in L^1(\mathbb{R}^N) + L^{N/\alpha}(\mathbb{R}^N) \quad \text{for some} \quad 0 < \alpha < N, \tag{93}$$

where $Z > 0$,

$$W \geqq 0 \text{ a.e.}; \quad \forall \varepsilon > 0, \left(W - \frac{1+\varepsilon}{|x|^\beta}\right)^+ \in L^1(\mathbb{R}^N) + L^{N/\beta}(\mathbb{R}^N) \quad \text{for some} \quad \alpha \leqq \beta < N. \tag{94}$$

Finally, f is an odd continuous C^1 function on $\mathbb{R}$ such that $f(0)=f'(0)=0$ and

$$|f'(t)|=o(t^{4/N}) \quad \text{as} \quad t\to\infty, \; f'(t)^+=o(t^{2\alpha/N}) \quad \text{as} \quad t\to 0, \tag{95}$$

$$f(t)\,t \geqq \int_0^t f(s)\,ds \quad \text{for all} \quad t\in\mathbb{R}. \tag{96}$$

We may then prove the

Theorem IV.3. *Assume* (93)–(96) *and* $Z\geqq\lambda$ *if* $\beta=\alpha$. *Then, there exists a sequence* $(\varphi_k)_{k\geqq 1}$ *of distinct solutions of* (92) *in* $H^1(\mathbb{R}^3)$ *such that* $\int_{\mathbb{R}^3}|\varphi_k|^2\,dx=\lambda$, *the Lagrange multiplier* $-\varepsilon_k$ *is non-positive and negative if* $\beta>\alpha$ *or if* $\beta=\alpha$ *and* $Z>\lambda$. *Finally,* $\varepsilon_k \xrightarrow[k]{} 0$, $\varphi_k \xrightarrow[k]{} 0$ *in* $L^p(\mathbb{R}^3)$ *for* $2<p\leqq\infty$, $\nabla\varphi_k \xrightarrow[k]{} 0$ *in* $L^2(\mathbb{R}^3)$. □

Remark. The assumptions (93)–(94) may be considerably relaxed or modified: we chose this formulation to emphasize the role of the behaviours at infinity of V, W. If (95) is natural enough in view of various standard arguments (see also Sect. II.4), we are convinced that (96) may be extended at least to cover the case when $f(t)\,t\geqq 0$ on $\mathbb{R}$....

Appendix: The Concentration-Compactness Method Revisited

Our goal here is to make a few remarks on the concentration-compactness method [43, 44]. We begin with a few abstract comments and we thus follow the heuristic setting given in [43]: we consider a functional minimization problem of the form

$$I_\lambda=\operatorname{Inf}\{\mathscr{E}(u)/u\in H,\; J(u)=\lambda\}, \qquad \lambda>0,$$

where H is some functional space, $\mathscr{E}$, J are functionals with a few formal properties described in [43]. If one can define functionals at infinity $\mathscr{E}^\infty$, J^∞, one introduces the problem at infinity

$$I_\lambda^\infty=\operatorname{Inf}\{\mathscr{E}^\infty(u)/u\in H,\; J^\infty(u)=\lambda\}.$$

Then, the concentration-compactness principle states that a necessary and sufficient condition for the compactness of all minimizing sequences is

$$I_\lambda<I_\alpha+I_{\lambda-\alpha}^\infty, \qquad \forall\alpha\in[0,\lambda). \tag{S.1}$$

And, if the problem is translation invariant and thus $\mathscr{E}=\mathscr{E}^\infty$, $J=J^\infty$, $I_\lambda=I_\lambda^\infty$, a necessary and sufficient condition for the compactness of all minimizing sequences is

$$I_\lambda<I_\alpha+I_{\lambda-\alpha}, \qquad \forall\alpha\in(0,\lambda). \tag{S.2}$$

In other words (at least for locally compact problems, see [43] for more details) the only possible loss of compactness is when a minimizing sequence (u^n) breaks into several parts $u_1^n, u_2^n, \ldots, u_K^n$ for some $K\geqq 1$ (K is in general finite but may be in some problems infinite) which are essentially supported in sets whose distance goes to infinity and u_1^n, respectively $\tilde u_j^n=u_j^n(\cdot+y_j^n)$ for some $|y_j^n|\xrightarrow[n]{}\infty$ $(j\geqq 2)$, is a minimizing sequence of I_{α_1}, respectively, $I_{\alpha_j}^\infty$, for some $\alpha_1\geqq 0$, $\alpha_j>0$ for $j\geqq 2$ such that $\sum_{j=1}^{K} \alpha_j = \lambda, I_\lambda = I_{\alpha_1} + \sum_{j=2}^{K} I^\infty_{\alpha_j}$. In addition, either $\tilde{u}^n_j$ is "compact" or $\tilde{u}^n_j$ "vanishes" (see [43]) for all $j \geqq 2$, and in many cases vanishing is easily excluded. Of course, all this is a bit formal and needs to be justified on each problem.

We want to explain in this appendix why additional information on $u^n_1, \ldots, u^n_K$ are often available. In particular, we will show why (65) holds and precise results will be given on two examples. Roughly speaking, we claim that in order to analyze (S.1)–(S.2) and the behaviour of arbitrary minimizing sequences, we may only consider minimizing sequences (u^n) which are "almost minima" of I_λ (this will be analyzed in particular in terms of 2nd order positivity conditions) and satisfy

$$\mathscr{E}'(u^n) - \theta_n J'(u^n) \underset{n}{\longrightarrow} 0 \quad \text{in} \quad H^* \tag{A.1}$$

for some Lagrange multiplier θ_n. Furthermore, in many cases one can prove that u^n breaks (up to subsequences) in a finite number K of pieces which are all compact up to different translations. Of course the case of compact minimizing sequences corresponds to $K=1$ (one compact piece). Again roughly speaking, there exist $\alpha_1 \geqq 0$, $\alpha_2, \ldots, \alpha_K > 0$ such that $I_{\alpha_1} + \sum_{j=2}^{K} I^\infty_{\alpha_j} = I_\lambda$, $\alpha_1 + \sum_{j=2}^{K} \alpha_j = \lambda$ $\left(\text{and thus } I_{\alpha_1} + \sum_{j\in J} I^\infty_{\alpha_j} = I_{\alpha_1+\beta} + \sum_{j\in J} \alpha_j,\ \sum_{j\in J} I^\infty_{\alpha_j} = I^\infty_\beta \sum_{j\in J} \alpha_j \text{ for any subset } J \text{ of } \{2, \ldots, K\} \text{ with } \beta = \sum_{j\in J} \alpha_j\right)$ and there exist u_1 minimum of I_{α_1} ($u_1 \equiv 0$ if $\alpha_1 = 0$), $\tilde{u}_j$ minima of I_{α_j} for $2 \leqq j \leqq K$ and sequences $(y^n_j)_n \in \mathbb{R}^N$ for $2 \leqq j \leqq k$, such that $|y^n_j| \underset{n}{\longrightarrow} \infty$, $|y^n_j - y^n_k| \underset{n}{\longrightarrow} \infty$ for $2 \leqq j \leqq K$, or $2 \leqq j < k \leqq K$ and

$$u^n - \sum_{j=2}^{K} \tilde{u}_j(\cdot - y^n_j) - u_1 \underset{n}{\longrightarrow} 0 \quad \text{in} \quad H. \tag{A.2}$$

In addition, if θ_n (or a subsequence) converges to θ, then $u_1, \tilde{u}_j$ for $2 \leqq j \leqq K$ satisfy

$$\mathscr{E}'(u_1) = \theta J'(u_1),\ (\mathscr{E}^\infty)'(\tilde{u}_j) = \theta (J^\infty)'(\tilde{u}_j) \quad \text{for} \quad i \geqq 2. \tag{A.3}$$

In other words, this means that *in order to check* (S.1) *or* (S.2) (at least in good cases when vanishing is easily excluded) one has to show strict subadditivity conditions for a *finite decomposition* for which minima exist and satisfy (A.3), i.e. the associated Euler-Lagrange equations but with the *same Lagrange multiplier*.

We begin with a few simple abstract remarks on the sufficiency of minimizing sequences satisfying (A.1). Indeed, by Ekeland's result [22], we know that for every minimizing sequence $(\tilde{u}^n)_n$, there exists $(u^n)_n$ such that

$$J(u^n) = \lambda,\ u^n - \tilde{u}^n \overset{n}{\longrightarrow} 0 \quad \text{in } H,\ \mathscr{E}(v) + \varepsilon_n \|v - u^n\|_H \geqq \mathscr{E}(u^n) \quad \forall v \in H,\ J(v) = \lambda \tag{A.4}$$

for some $\varepsilon_n > 0$, $\varepsilon_n \underset{n}{\longrightarrow} 0$. Obviously, it is enough to analyze the behaviour of $(u^n)_n$. Now, if $\mathscr{E}, J$ are differentiable at u^n this implies

$$\| \mathscr{E}'(u^n) - \theta_n J'(u^n) \|_{H^*} \leqq \varepsilon_n, \tag{A.5}$$

while if $\mathscr{E}$, J are uniformly twice differentiable on bounded sets (or on minimizing sequences) we also deduce for some $\gamma_n > 0$, $\gamma_n \xrightarrow[n]{} 0$,

$$\mathscr{E}''(u^n)(\psi,\psi) - \theta_n J''(u^n)(\psi,\psi) + \gamma_n \|\psi\|^2 \geqq 0 \tag{A.6}$$

for all $\psi \in H$ such that $\langle J'(u^n), \psi\rangle = 0$ [in fact one needs considerably less regularity on $\mathscr{E}$ and J in order to derive (A.6)...].

Next, in order to make rigorous the above considerations, we will consider two examples. The first one is the one considered in Corollary II.2 [see (65)]

Example 1. We choose $J(u) = \int_{\mathbb{R}^3} |u|^2\,dx$, $\mathscr{E}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + V|u|^2 + F(u)\,dx + \frac{1}{2}D(|u|^2, |u|^2)$, where F satisfies the conditions used in part ii) of Corollary II.2. Assuming $Z \geqq \lambda$, we show the above decomposition of a minimizing sequence, i.e. we show (65), completing thus the proof of Corollary II.2 □

Example 2. We choose $J(u) = \int_{\mathbb{R}^3} |u|^2\,dx$, $\mathscr{E}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{a}{p}|u|^{2p}\,dx + -\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} |u|^2(x)\,|u|^2(y)\,V(x-y)\,dx\,dy$, where $a>0$, $p>2$, and V is a given potential that we assume to be nonnegative, spherically symmetric, nonincreasing with respect to $|x|$ and $V \in L^1(\mathbb{R}^3) + L^\beta(\mathbb{R}^3)$ for some $\beta < \infty$, $V \not\equiv 0$. In this example, we assume that $\lambda > 0$ is such that $I_\lambda < 0$. Of course, we choose the space here to be $H^1(\mathbb{R}^3)$ if $p \leqq 3$ and $H^1(\mathbb{R}^3) \cap L^{2p}(\mathbb{R}^3)$ if $p \geqq 3$.

Before stating the result we want to prove, let us briefly discuss the assumption on I_λ. By a simple scaling argument one sees that $I_\lambda \leqq 0$ always holds for all $\lambda > 0$. And we claim there exists $\lambda_0 \in [0,\infty)$ such that $I_\lambda < 0$ if $\lambda > \lambda_0$ (λ_0 only depends on V): indeed there exist $R < \infty$, $\varphi \in \mathscr{D}(\mathbb{R}^3)$ such that

$$\frac{1}{2}\left(\int_{B_R} V\,dx\right)\left(\int_{\mathbb{R}^3} |\varphi|^4\,dx\right) > \frac{a}{p}\left(\int_{\mathbb{R}^3} |\varphi|^{2p}\,dx\right),$$

then we compute for $\sigma > 0$,

$$\begin{aligned}\mathscr{E}\left(\varphi\left(\frac{\cdot}{\sigma}\right)\right) &\leqq \sigma \int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx + \sigma^3 \frac{a}{p}\int_{\mathbb{R}^3} |\varphi|^{2p}\,dx \\ &\quad - \sigma^6 \iint_{\mathbb{R}^3\times\mathbb{R}^3} |\varphi(x)|^2\,|\varphi(y)|^2\,V(\sigma(x-y))\,1_{(\sigma|x-y|\leqq R)}\,dx\,dy \\ &= \sigma \int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx + \sigma^3\left[\frac{a}{p}\int_{\mathbb{R}^3} |\varphi|^{2p}\,dx \right. \\ &\quad \left. -\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} |\varphi(x)|^2\,|\varphi(y)|^2\,\sigma^3\,V^R(\sigma(x-y))\,dx\,dy\right],\end{aligned}$$

where $V^R(x) = V(x)\,1_{|x|\leqq R}$. Remarking that

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} |\varphi(x)|^2\,|\varphi(y)|^2\,\sigma^3\,V^R(\sigma(x-y))\,dx\,dy \xrightarrow[\sigma\to\infty]{} \left(\int_{B_R} V\,dx\right)\left(\int_{\mathbb{R}^3} |\varphi|^4\,dx\right),$$

we conclude that $\mathscr{E}\left(\varphi\left(\frac{\cdot}{\sigma}\right)\right) < 0$ for σ large enough, proving thus our claim.

In the case of Example 2, we want to show how minimizing sequences satisfying (A.1) can be decomposed as in (A.2), (A.3) with the conditions on u_1, $\tilde{u}_j$ given before (A.2), (A.3). Notice of course that in the Example 2 we have $\mathscr{E}=\mathscr{E}^\infty$, $J=J^\infty$. Finally, let us mention that we are only interested in the compactness up to translations of minimizing sequences since the problem is translation invariant (i.e. either $K=1$, or $K=2$ and $u_1\equiv 0$). The implications of such decompositions in Example 2 will be discussed elsewhere.

On these two examples we consider minimizing sequences u^n which satisfy (A.1) [or (A.5) and (A.6)]. Of course, u^n is bounded in H and in the two examples the Lagrange multiplier $\theta_n=\langle \mathscr{E}'(u^n), u^n\rangle$ remains bounded. Therefore we may assume without loss of generality that $\theta_n \xrightarrow[n]{} \theta$.

Step 1. We show that θ_n remains negative and bounded away from 0, i.e.

$$\exists v>0, \quad \theta_n \leqq -v<0. \tag{A.7}$$

In the case of Example 1, this is proved in Sect. II.4 using (A.6). In the case of Example 2, we argue as follows. Introducing as in [43, 44] the concentration function of $|u^n|^2$, i.e.

$$Q_n(t)=\sup_{y\in \mathbb{R}^3} \int_{y+B_t} |u^n|^2\,dx, \quad \text{for} \quad t\geqq 0,$$

we see that up to subsequences, and we will in fact neglect all the extractions of subsequences in the arguments below, either $Q_n(t)\xrightarrow[n]{} 0$ for all $t<\infty$ or there exists $\alpha>0$ such that $Q_n(t_0)\geqq\alpha>0$ for $n\geqq 1$ and for some $t_0>0$. In the first case (vanishing with the terminology of [43, 44]) then we know by [43] that u^n converges strongly to 0 in $L^q(\mathbb{R}^3)$ for $2<q<\max(6,2p)$. This implies easily

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} |u^n|^2(x)\,|u^n|^2(y)\,V(x-y)\,dx\,dy \xrightarrow[n]{} 0,$$

hence $I_\lambda\geqq 0$. We reach a contradiction since we assumed $I_\lambda<0$. Therefore, there exist $\alpha>0$, $y_n\in\mathbb{R}^3$ such that

$$\int_{y_n+B_{t_0}} |u^n|^2\,dx \geqq \alpha>0.$$

We then consider the sequence $\tilde{u}^n=u^n(\cdot+y_n)$ which is still a minimizing sequence satisfying (A.1) with the same Lagrange multiplier θ_n. Using for instance the concentration-compactness arguments, we see that $\tilde{u}^n$ converges weakly in H to some $\tilde{u}$ which is a minimum of $I_{\tilde{\alpha}}$, where $\tilde{\alpha}=\int_{\mathbb{R}^3}|\tilde{u}|^2\,dx\in(0,\lambda]$ (using some specific properties of $\mathscr{E}$ here we may also observe that

$$\mathscr{E}(\tilde{u}^n)-(\mathscr{E}(\tilde{u}^n-\tilde{u})+\mathscr{E}(\tilde{u}))\xrightarrow[n]{} 0,$$

$$\int_{\mathbb{R}^3}|\tilde{u}^n-\tilde{u}|^2\,dx\xrightarrow[n]{}\lambda-\tilde{\alpha}, \quad \varliminf_n \mathscr{E}(\tilde{u}^n-\tilde{u})\geqq I_{\lambda-\tilde{\alpha}},$$

and since $I_\lambda\leqq I_{\tilde{\alpha}}+I_{\lambda-\tilde{\alpha}}$ we obtain the above claim easily). It is also a standard exercise to pass to the limit in (A.1), and we obtain

$$-\Delta\tilde{u}+a|\tilde{u}|^{2p-2}\tilde{u}-(V*|\tilde{u}|^2)\tilde{u}-\theta\tilde{u}=0 \quad \text{in} \quad \mathbb{R}^3. \tag{A.8}$$

Furthermore, since $\tilde{u}$ is a minimum of $I_{\tilde{\alpha}}$, using a standard symmetrization argument one deduces that $\pm\tilde{u}$ (say $\tilde{u}$) is radial, nonnegative and nonincreasing. We want to prove that $\theta<0$, and we argue by contradiction. Assume that $\theta \geqq 0$. We claim that there exists $\gamma>0$ such that for large $|x|$

$$V*|\tilde{u}|^2 \geqq \gamma |\tilde{u}|^2 .$$

Indeed since $V \not\equiv 0$ and V is radial, we can find $\delta>0$, $R<\infty$ such that

$$\int_{(z_1 \geqq \delta, |z| \leqq R)} V(z)\, dz \geqq \gamma > 0 .$$

Then, for $|x| \geqq \frac{R^2}{2\delta}$, we observe that $V*|\tilde{u}|^2(x) = V*|\tilde{u}|^2(\bar{x})$ with $\bar{x}=|x|e_1$,

$$\begin{aligned} V*|\tilde{u}|^2 &\geqq \Bigg(\int_{|y|\leqq|\bar{x}|} V(\bar{x}-y)\, dy \Bigg) |\tilde{u}(\bar{x})|^2 \\ &= \Bigg(\int_{(|z|^2 \leqq 2z_1|x|)} V(z)\, dz \Bigg) |\tilde{u}(x)|^2 \\ &\geqq \Bigg(\int_{(z_1 \geqq \delta, |z| \leqq R)} V(z)\, dz \Bigg) |\tilde{u}(x)|^2 \geqq \gamma |\tilde{u}(x)|^2 . \end{aligned}$$

Therefore, for $|x|$ large we find

$$-\Delta\tilde{u} \geqq \gamma\tilde{u}^3 + |\theta|\tilde{u} - a\tilde{u}^{2p-1} \geqq 0, \qquad \tilde{u} \geqq 0 \quad \text{on } \mathbb{R}^3,$$

since $p>2$ and $\tilde{u}\to 0$ as $|x|\to\infty$. This yields

$$\tilde{u}(x) \geqq \frac{\mu}{|x|} \quad \text{for } |x| \text{ large and for some } \mu>0,$$

contradicting the fact that $\tilde{u}\in L^2(\mathbb{R}^3)$. Hence, $\theta<0$ and (A.7) is proved for n large (that we take below equal to 1). □

Step 2. We now want to prove two related properties. The first one is the following: let $u \in H$ satisfy $\int_{\mathbb{R}^3} |\nabla u|^2\, dx \leqq C_0$ for some fixed constant C_0 and

$$-\Delta u - \theta u - \theta u + B(u) = 0 \quad \text{in } \mathbb{R}^3, \tag{A.9}$$

where $\theta<0$, $B(u) = \left(|u|^2 * \frac{1}{|x|}\right) u + f(u)$ in Example 1, $B(u) = a|u|^{2p-2}u - (|u|^2 * V)u$ in Example 2. Then, there exists $\varepsilon_0>0$ depending only on $|\theta|$, C_0 such that

$$\int_{\mathbb{R}^3} |u|^2\, dx \leqq \varepsilon_0 \Rightarrow u \equiv 0 . \tag{A.10}$$

To prove this claim we may argue by contradiction considering a sequence $(u_n)_n$ satisfying the above conditions and such that $\int_{\mathbb{R}^3} |u_n|^2\, dx \xrightarrow[n]{} 0$, $u_n \not\equiv 0$. We first observe that u_n also converges to 0 in $L^\infty(\mathbb{R}^3)$: one just has to use standard regularity theory for second-order elliptic equations and the various assumptions we made on the nonlinear terms. Next, because of (A.9) we find

$$\|u_n\|_{L^2(\mathbb{R}^3)} \leqq C(|\theta|)\, \|f^-(u_n)\|_{L^2(\mathbb{R}^3)} \qquad \text{in Example 1},$$

$$\|u_n\|_{L^2(\mathbb{R}^3)} \leqq C(|\theta|)\, \|(|u_n|^2 * V)u_n\|_{L^2(\mathbb{R}^3)} \qquad \text{in Example 2}.$$

In both examples, the upper bound may be majorized by $\varepsilon_n \|u_n\|_{L^2(\mathbb{R}^3)}$, where $\varepsilon_n \xrightarrow[n]{} 0$, and we reach the desired contradiction.

The second property enables us to exclude some vanishing phenomena: let v_n be a bounded sequence in H satisfying (A.1), where θ_n satisfies (A.7). Then, if $|v_n|^2$ vanishes, i.e.

$$\operatorname*{Sup}_{y\in\mathbb{R}^3} \int_{y+B_R} |v_n|^2\,dx \xrightarrow[n]{} 0 \quad \text{for all} \quad R<\infty\,,$$

then v_n converges strongly in H to 0.

Indeed, we know by [43] that v_n converges strongly in $L^q(\mathbb{R}^3)$ to 0 for $2<q<\max(6,2p)$. Then multiplying (A.1) by v_n, we deduce

$$\|v_n\|^2_{H^1(\mathbb{R}^3)} \leqq C\varepsilon_n \|v_n\|_{H^1(\mathbb{R}^3)} + C\|f^-(v_n)\|_{H^{-1}(\mathbb{R}^3)} \qquad \text{in Example 1},$$

$$\|v_n\|^2_{H^1(\mathbb{R}^3)} + \|v_n\|^{2p}_{L^{2p}(\mathbb{R}^3)} \leqq C\varepsilon_n [\|v_n\|_{H^1(\mathbb{R}^3)} + \|v_n\|_{L^{2p}(\mathbb{R}^3)}] + C\|(|v_n|^2 * V)\,v_n\|_{H^{-1}(\mathbb{R}^3)} \qquad \text{in Example 2},$$

where $\varepsilon_n>0$, $\varepsilon_n \xrightarrow[n]{} 0$. Next, we observe

$$\begin{aligned}\|f^-(v_n)\|_{H^{-1}(\mathbb{R}^3)} &\leqq C\|f^-(v_n)\,1_{|v_n|\leqq\varepsilon}\|_{L^2(\mathbb{R}^3)} \\ &\quad + C\|f^-(v_n)\,1_{|v_n|\geqq 1/\varepsilon}\|_{L^{6/5}(\mathbb{R}^3)} + C_\varepsilon \||v_n|^2\|_{L^2(\mathbb{R}^3)} \\ &\leqq \delta(\varepsilon)\,[\|v_n\|_{L^2(\mathbb{R}^3)} + \|v_n\|^5_{L^6(\mathbb{R}^3)}] + C_\varepsilon \|v_n\|^2_{L^4(\mathbb{R}^3)}\end{aligned}$$

in Example 1 with $\delta(\varepsilon)\to 0$ as $\varepsilon\to 0$, while in Example 2 we have

$$\|(|v_n|^2 * V)\,v_n\|_{H^{-1}(\mathbb{R}^3)} \leqq C\|v_n\|^3_{L^{\bar p}} + C\|v_n\|^3_{L^{\bar q}}$$

for some $\bar p$, $\bar q$ satisfying $2<\bar p<\bar q<6$.

We may now deduce from all these ad hoc bounds the convergence of v_n to 0 in H. In fact, we only used the existence of some $t>0$ such that $Q_n(t)\to 0$. □

Step 3. Extraction of the local part in Example 1. In the remaining steps we will prove the decompositions we announced by an argument which will use the fact in particular that the functional $\int_{\mathbb{R}^3} |\nabla u|^2\,dx$ is quadratic: this will allow us to use only weak limits, while for more general problems one has to use more systematically the concentration functions as in [43] to perform the various dichotomies. In the case of Example 1, we consider the weak limit u_1 of u^n (or a subsequence) in $H^1(\mathbb{R}^3)$: if $u_1\equiv 0$ there is nothing to do. If $u_1\not\equiv 0$, i.e. $\alpha_1=\int_{\mathbb{R}^3}|u_1|^2\,dx\in(0,\lambda]$, we consider $\tilde u^n = u^n - u_1$. Obviously, $\int_{\mathbb{R}^3}|\tilde u^n|^2\,dx \xrightarrow[n]{} \lambda-\alpha_1$ while

$$\begin{aligned}\mathscr{E}(u^n) = \mathscr{E}(u_1+\tilde u^n) &= \mathscr{E}(u_1) + \mathscr{E}^\infty(\tilde u^n) + \varepsilon_n + \int_{\mathbb{R}^3} V|\tilde u^n|^2\,dx \\ &\quad + 2D(|u_1|^2, u_1\tilde u^n) + D(|u_1|^2, |\tilde u^n|^2) + 2D(|\tilde u^n|^2, u_1\tilde u^n) \\ &\quad + \int_{\mathbb{R}^3} F(u_1+\tilde u_n) - F(u_1) - F(\tilde u^n)\,dx,\end{aligned}$$

where $\varepsilon_n \underset{n}{\longrightarrow} 0$. Next, we observe that

$$\int_{\mathbb{R}^3} V|\tilde{u}^n|^2 dx \underset{n}{\longrightarrow} 0, \quad u_1 \tilde{u}^n \underset{n}{\longrightarrow} 0 \quad \text{in} \quad L^q(\mathbb{R}^3) \quad \text{for} \quad 1 \leqq q \leqq 3,$$
$$D(|u_1|^2, |\tilde{u}^n|^2) \underset{n}{\longrightarrow} 0,$$

hence we deduce

$$\mathscr{E}(u^n) - \mathscr{E}(u_1) - \mathscr{E}^\infty(\tilde{u}^n) - \int_{\mathbb{R}^3} F(u_1 + \tilde{u}^n) - F(u_1) - F(\tilde{u}^n)\, dx \underset{n}{\longrightarrow} 0.$$

We claim that this last integral goes to 0 as n goes to ∞. Indeed, by the assumptions made on F we have

$$\int_{B_R} |F(u_1 + \tilde{u}^n) - F(u_1)|\, dx \underset{n}{\longrightarrow} 0, \quad \int_{B_R} |F(\tilde{u}^n)|\, dx \underset{n}{\longrightarrow} 0$$

for all $R < \infty$, while we have obviously $\int_{B_R^c} |F(u_1)|\, dx \to 0$ as $R \to \infty$ and

$$\int_{B_R^c} |F(u_1 + \tilde{u}^n) - F(\tilde{u}^n)|\, dx \leqq C \int_{B_R^c} \{|u_1| + |\tilde{u}^n| + |u_1|^5 + |\tilde{u}^n|^5\} |u_1|\, dx;$$

therefore $\int_{B_R^c} |F(u_1 + \tilde{u}^n) - F(\tilde{u}^n)|\, dx \to 0$ as $R \to \infty$, uniformly in n and our claim is proved. In conclusion, we have shown that

$$\mathscr{E}(u^n) - \{\mathscr{E}(u_1) + \mathscr{E}^\infty(\tilde{u}^n)\} \underset{n}{\longrightarrow} 0, \tag{A.11}$$

and since $\mathscr{E}(u^n) \underset{n}{\longrightarrow} I_\lambda$, $\mathscr{E}(u_1) \geqq I_{\alpha_1}$, $\underset{n}{\underline{\lim}}\, \mathscr{E}^\infty(\tilde{u}^n) \geqq I^\infty_{\lambda-\alpha_1}$ and $I_\lambda \leqq I_{\alpha_1} + I^\infty_{\lambda-\alpha_1}$, we deduce that u_1 is a minimum of I_{α_1} and $\tilde{u}^n$ is a minimizing sequence of $I^\infty_{\lambda-\alpha_1}$.

In addition, by an easy passage to the limit, we see that u_1 satisfies

$$-\Delta u_1 + V u_1 + \left(|u_1|^2 * \frac{1}{|x|}\right) u_1 + f(u_1) - \theta u_1 = 0 \quad \text{in} \quad \mathbb{R}^3. \tag{A.12}$$

Our last claim for this step is that $\tilde{u}^n$ satisfies

$$-\Delta \tilde{u}^n + \left(|\tilde{u}^n|^2 * \frac{1}{|x|}\right) \tilde{u}^n + f(\tilde{u}^n) - \theta \tilde{u}^n \underset{n}{\longrightarrow} 0 \quad \text{in} \quad H^{-1}(\mathbb{R}^3) \tag{A.13}$$

(i.e. $(\mathscr{E}^\infty)'(\tilde{u}^n) - \theta (J^\infty)'(\tilde{u}^n) \underset{n}{\longrightarrow} 0$ in H^{-1}).

Indeed, subtracting (A.12) from (A.1) we get

$$-\Delta \tilde{u}^n + \left(|\tilde{u}^n|^2 * \frac{1}{|x|}\right) \tilde{u}^n + f(\tilde{u}^n) - \theta \tilde{u}^n + T_n \underset{n}{\longrightarrow} 0 \quad \text{in} \quad H^{-1}(\mathbb{R}^3),$$

where

$$T_n = V\tilde{u}^n + f(u^n) - (f(u_1) + f(\tilde{u}^n)) + \left(|u^n|^2 * \frac{1}{|x|}\right) u^n$$
$$+ - \left(\left(|u_1|^2 * \frac{1}{|x|}\right) u_1 + \left(|\tilde{u}^n|^2 * \frac{1}{|x|}\right) \tilde{u}^n\right).$$

And we prove exactly as before that $T_n \xrightarrow[n]{} 0$ in $H^{-1}(\mathbb{R}^3)$: for instance we will treat only one term in T_n, namely the difference

$$f(u^n) - [f(u_1) + f(\tilde{u}^n)].$$

From the assumptions made on f, one deduces easily that for all $R < \infty$,

$$1_{B_R}(f(u^n) - f(u_1)) \xrightarrow[n]{} 0, \quad 1_{B_R} f(\tilde{u}^n) \xrightarrow[n]{} 0 \quad \text{in} \quad H^{-1}(\mathbb{R}^3),$$

while

$$1_{B_R^c} f(u_1) \to 0 \quad \text{in} \quad H^{-1}(\mathbb{R}^3) \quad \text{as} \quad R \to \infty,$$

and

$$|1_{B_R^c}\{f(u^n) - f(\tilde{u}^n)\}| \leqq C 1_{B_R^c}(1 + |u_1|^4 + |\tilde{u}^n|^4)|u_1|.$$

We may now conclude, since

$$1_{B_R^c}|u_1| \to 0 \quad \text{in } L^2(\mathbb{R}^3) \quad \text{as} \quad R \to \infty,$$

$$1_{B_R^c}(|u_1|^5 + |u_1||\tilde{u}^n|^4) \to 0 \quad \text{in} \quad L^{6/5}(\mathbb{R}^3) \quad \text{as} \quad R \to \infty, \quad \text{uniformly in } n.$$

Step 4. Conclusion. We now argue on the sequence $\tilde{u}^n$ in Example 1 and u^n in Example 2. For these sequences we consider the concentration functions $Q_n(t)$ of respectively $|\tilde{u}^n|^2$, $|u^n|^2$. In view of Step 2, $|\tilde{u}^n|^2$, $|u^n|^2$ cannot vanish (or if this happens in Example 1, this implies $\tilde{u}^n \xrightarrow[n]{} 0$ in $L^2(\mathbb{R}^3)$ and we stop the decomposition) i.e. there exist $t_0 > 0$, $\gamma > 0$ such that

$$Q_n(t_0) \geqq \gamma > 0.$$

This means there exists $(y_n)_n$ in $\mathbb{R}^3$ such that

$$\int_{y_n + B_{t_0}} |\varphi^n|^2 \, dx \geqq \gamma > 0,$$

where $\varphi^n = \tilde{u}^n$ in Example 1, $= u^n$ in Example 2.

And we may consider $\psi^n = \varphi^n(y_n + \cdot)$ which will converge weakly (up to subsequences) in H to some u_2. Obviously,

$$0 < \int_{\mathbb{R}^3} |u_2|^2 \, dx = \alpha_2 \leqq \lambda - \alpha_1 \quad \text{in Example 1}, \leqq \lambda \text{ in Example 2}.$$

Furthermore, one has obviously in Example 1, $|y_n| \xrightarrow[n]{} \infty$. By the same argument as in Step 3, we deduce in both examples

$$\mathscr{E}^\infty(\psi^n) - [\mathscr{E}^\infty(u_2) + \mathscr{E}^\infty(\psi^n - u_2)] \xrightarrow[n]{} 0,$$

$$u_2 \text{ is a minimum of } I_{\alpha_2}^\infty, \quad \mathscr{E}^\infty(\psi^n - u_2) \xrightarrow[n]{} I_{\beta_2}^\infty,$$

$$\int_{\mathbb{R}^3} |\psi^n - u_2|^2 \, dx \xrightarrow[n]{} \beta_2,$$

where $\beta_2 = \lambda - \alpha_1 - \alpha_2$ in Example 1, $= \lambda - \alpha_2$ in Example 2. In addition,

$$(\mathscr{E}^\infty)'(u_2) - \theta u_2 = 0 \qquad \text{in } \mathbb{R}^3,$$
$$(\mathscr{E}^\infty)'(\psi^n - u_2) - \theta(\psi^n - u_2) \underset{n}{\longrightarrow} 0 \qquad \text{in } H,$$

where $\mathscr{E}^\infty = \mathscr{E}$ in Example 2.

The only new arguments concern the following facts:

$$\int_{\mathbb{R}^3} \big|\, |\psi^n|^{2p} - |u_2|^{2p} - |\psi^n - u_2|^{2p} \big|\, dx \underset{n}{\longrightarrow} 0$$

$$|\psi^n|^{2p-2}\psi^n - |u_2|^{2p-2}u_2 - |\psi^n - u_2|^{2p-2}(\psi^n - u_2) \underset{n}{\longrightarrow} 0 \quad \text{in } L^{\frac{2p}{2p-1}},$$

the first convergence is a consequence of Brézis and Lieb's lemma [17] while the second one is closely related. Indeed one just needs to observe that for each $\varepsilon > 0$, there exists $C_\varepsilon < \infty$ such that for all $x, y \in \mathbb{R}$,

$$\big|\, |x+y|^{2p-2}(x+y) - |x|^{2p-2}x - |y|^{2p-2}y \,\big| \leqq \varepsilon |y|^{2p-1} + C_\varepsilon |x|^{2p-1},$$

and that the second quantity above converges a.e. to 0.

At this stage, we consider $(\psi^n - u_2)$, and we reiterate the above arguments. This iterative decomposition stops after a finite number of times, since by Step 2 we know that $\alpha_2, \alpha_3, \alpha_4 \dots$ remain bounded from below by a fixed positive constant. Hence, we obtain some integer L and positive constants $\alpha_2, \dots, \alpha_L$ such that there exist $u_2, \dots, u_L$ minima of $I^\infty_{\alpha_1}, \dots, I^\infty_{\alpha_2}$, satisfying in addition,

$$(\mathscr{E}^\infty)'(u_i) - \theta u_i = 0 \quad \text{in } \mathbb{R}^3, \quad \int_{\mathbb{R}^3} |u_i|^2\, dx = \alpha_i,$$

and $I_\lambda = I_{\alpha_1} + \sum_{j=2}^{L} I^\infty_{\alpha_j}$, $\lambda = \sum_{i=1}^{L} \alpha_i$ in Example 1, while $I_\lambda = \sum_{j=2}^{L} I^\infty_{\alpha_j}$, $\lambda = \sum_{j=2}^{L} \alpha_j$ in Example 2. Furthermore, there exist sequences $(y_n^j)_n$ in $\mathbb{R}^3$ for $2 \leqq j \leqq L$ satisfying

$$|y_n^i - y_n^j| \underset{n}{\longrightarrow} \infty \qquad \text{for } 2 \leqq i < j \leqq L$$

and $v^n = u^n - u_1 - \sum_{j=2}^{L} u_j(\cdot - y_n^j) \underset{n}{\longrightarrow} 0$ in $H^1(\mathbb{R}^3)$, $|y_n^j| \underset{n}{\longrightarrow} \infty$ in Example 1, while $v^n = u^n - \sum_{j=2}^{L} u_j(\cdot - y_n^j) \underset{n}{\longrightarrow} 0$ in H in Example 2.

Remark. We point out that the above arguments are somewhat related to those used in Brézis and Coron [16], Struwe [56]....

In an attempt to explain a bit the above arguments, we want to conclude this appendix by a general decomposition lemma, in the spirit of the first concentration-compactness lemma in [43, 44].

Lemma 1. *Let $k \geqq 1$ and let $(P_n)_n$ be a sequence of probability measures in $\mathbb{R}^k$. Then there exists a subsequence of P_n that we still denote by P_n (to simplify) which satisfies the following properties: one can find M in $\mathbb{N} \cup \{+\infty\}$ and sequences $(y_n^1)_n$ in $\mathbb{R}^k$, positive numbers α_i for $1 \leqq i < M$ such that*

$$\alpha_1 \geqq \alpha_2 \geqq \dots, \quad \sum_i \alpha_i \leqq 1, \tag{A.14}$$

$$|y_n^i - y_n^j| \underset{n}{\longrightarrow} \infty \quad \textit{for} \quad i \neq j, \tag{A.15}$$

$$P_n\left(B(y_n^i, R_n^i) \Big\backslash \bigcup_{1 \leq j \leq i-1} B(y_n^j, R_n^j)\right) \underset{n}{\longrightarrow} \alpha_i,$$

$$\textit{for some sequences} \quad R_n^i \underset{n}{\longrightarrow} \infty, \quad \forall i, \tag{A.16}$$

$$\forall i \geqq 1, \quad \forall \varepsilon > 0, \quad \exists R < \infty, \quad P_n\left(B(y_n^i, R) \Big\backslash \bigcup_{1 \leq j \leq i-1} B(y_n^j, R_n^j)\right) \geqq \alpha_i - \varepsilon \quad \forall n \geqq 1, \tag{A.17}$$

$$1_{A_n} P_n \quad \textit{vanishes}, \text{ i.e. } \sup_{y \in \mathbb{R}^k} P_n(B(y, R) \cap A_n) \underset{n}{\longrightarrow} 0, \quad \forall R < \infty, \tag{A.18}$$

where $A_n = \bigcap_i (\mathbb{R}^k \backslash B(y_n^i, R_n^i))$.

Remarks. i) The case $M = 0$ corresponds to the case when P_n itself vanishes. The case $M = 1$, $\alpha_1 = 1$ corresponds to the case when P_n is tight up to the translation y_n^1. Finally, the remaining case in [41, 42] namely dichotomy, corresponds to $M \geqq 2$. Then, we split P_n in two parts,

$$P_n^1 = 1_{B(y_n^1, \tilde{R}_n^1)} P_n, \quad \text{where} \quad \tilde{R}_n^1 \leqq R_n^1 \quad \text{and} \quad \frac{\tilde{R}_n^1}{R_n^1} \underset{n}{\longrightarrow} 0, \quad \tilde{R}_n^1 \underset{n}{\longrightarrow} \infty$$

[observe that (A.16) and (A.18) still hold with R_n^1 replaced by $\tilde{R}_n^1$] and

$$P_n^2 = 1_{B(y_n^1, R_n^1)^c} P_n.$$

i) The above proof may now be interpreted in the light of this simple general lemma (in fact, this lemma may be used to present another proof slightly more technical but also more general as we explain below). First of all, we may apply the above lemma with $P_n = |u^n|^2$ or $P_n = |u^n|^2 + |\nabla u^n|^2$ (or even $P_n = |u^n|^2 + |\nabla u^n|^2 + |u^n|^{2p}$ in Example 2) – we neglect the fact that P_n is not a probability measure, just replace P_n by $P_n / P_n(\mathbb{R}^3)$. Then, roughly speaking, each piece u_i of the above decomposition is the weak limit in H of $u^n(y_n^i + \cdot)$. And the fact that M is finite or that the decomposition yields a strong convergence in H to 0 are consequences of (A.14) and (A.18) combined with the crucial argument given in Step 2 [and Step 2 is the only place where we used the information (A.7)]. Indeed if $M = +\infty$, then $\alpha_i \underset{i}{\longrightarrow} 0$ because of (A.14), and u_i satisfies the Euler-Lagrange equation together with (for instance) $\int_{\mathbb{R}^3} |u_i|^2 \, dx = \alpha_i$, and we reach a contradiction with Step 2. All possibilities of vanishing (P_n vanishes or $1_{A_n} P_n$ vanishes) are also excluded because of Step 2. And we obtain $P_n(A_n) \underset{n}{\longrightarrow} 0$, which implies the strong convergence in H.

As we said before, this lemma may be used to construct differently u_i (adding some information to the mere information of weak limits which is too weak for general problems with less "quadratic" structure: recall that in an Hilbert space, if $x_n \rightharpoonup x$, then $|x_n - x|^2 + |x|^2 - |x_n|^2 \underset{n}{\longrightarrow} 0$): indeed, it is possible to consider directly

$$\chi((y_n^i + \cdot)/\tilde{R}_n^i) \, u^n(y_n^i + \cdot),$$

where χ is some cut-off function, $\tilde{R}_n^i \leqq R_n^i$, $\tilde{R}_n^i \xrightarrow[n]{} \infty$, $\frac{\tilde{R}_n^i}{R_n^i} \xrightarrow[n]{} 0$. Another way to "cut" is also given in [45].

Let us also finally mention that in many problems the information necessary to prove Step 2 [(A.7) here] is automatic.

Proof of Lemma 1. We are going to use systematically the concentration function $Q_n(t)$ of P_n, i.e.

$$Q_n(t) = \operatorname*{Sup}_{y \in \mathbb{R}^k} P_n(B(y, t)) \quad \text{for all} \quad t > 0.$$

We will not bother to extract subsequences, leaving to the reader the standard diagonal extractions. Now, with these notations and conventions we recall from [43] that either P_n vanishes and we conclude $M = 0$, or $Q_n(t) \xrightarrow[n]{} Q(t)$, $\forall t > 0$, where Q is nondecreasing and $Q \not\equiv 0$. Let $\alpha_1 = \lim_{t \uparrow +\infty} Q(t) > 0$. Obviously, $\alpha_1 \leqq 1$ and we deduce from Lemma 2 below that there exists $y_n^1 \in \mathbb{R}^k$ such that (A.16) and (A.17) hold for $i = 1$. We then consider $P_n^2 = 1_{B(y_n^1, R_n^1)^c} P_n$, and we introduce the concentration function Q_n^2 of P_n^2. Again, with our conventions, we may assume that either P_n^2 vanishes and the lemma is proved with $M = 1$, or that $Q_n^2(t) \xrightarrow[n]{} Q^2(t)$, $\forall t > 0$ for some nondecreasing function Q^2 and $Q^2 \not\equiv 0$. Let $\alpha_2 = \lim_{t \uparrow \infty} Q^2(t) > 0$.

We claim that $\alpha_2 \leqq \alpha_1$. Let us argue by contradiction: if $\alpha_2 > \alpha_1$, there exists $z_n \in \mathbb{R}^k$, $R < \infty$ such that

$$P_n^2(B(z_n, R)) \geqq \alpha_1 + \nu, \quad \text{for some} \quad \nu > 0.$$

Therefore, $P_n(B(z_n, R)) \geqq \alpha_1 + \nu$, and passing to the limit we obtain $Q(R) \geqq \alpha_1 + \nu$, contradicting the definition of α_1. Hence, $\alpha_2 \leqq \alpha_1$. Next, we can find using again Lemma 2 a sequence $y_n^2 \in \mathbb{R}^k$ such that (A.16) and (A.17) hold for $i = 2$. We next claim that $|y_n^1 - y_n^2| \xrightarrow[n]{} \infty$. Indeed, observe that (A.17) for $i = 2$ implies obviously that $y_n^2 \notin B\left(y_n^1, \frac{R_n^1}{2}\right)$ for n large, hence $|y_n^2 - y_n^1| \xrightarrow[n]{} \infty$. Finally, we show that $\alpha_1 + \alpha_2 \leqq 1$. This follows easily from (A.16)–(A.17) for $i = 1, 2$. Indeed, for all $\varepsilon > 0$ there exists $R_2 < \infty$ such that

$$P_n(B(y_n^2, R_2) \backslash B(y_n^1, R_n^1)) \geqq \alpha_2 - \varepsilon,$$

hence

$$P_n(B(y_n^2, R_2) \bigcup B(y_n^1, R_n^1)) \geqq \alpha_2 - \varepsilon + P_n(B(y_n^1, R_n^1)),$$

i.e. $1 \geqq \alpha_2 - \varepsilon + \alpha_1$, and we conclude.

Next, assume that we have built $P_n^2, \ldots, P_n^l$, $\alpha_1, \ldots, \alpha_l$, $y_n^1, \ldots, y_n^l$ satisfying (A.14)–(A.17) for $1 \leqq i \leqq l$. We then consider

$$P_n^{l+1} = 1_{B(y_n^l, R_n^l)^c} P_n^l$$

and its concentration function Q_n^{l+1}. Again, either P_n^{l+1} vanishes and the lemma is proved or $Q_n^{l+1}(t) \xrightarrow[n]{} Q^{l+1}(t)$, $\forall t > 0$ for some nondecreasing function Q^{l+1} and $Q^{l+1} \not\equiv 0$. We denote by $\alpha_{l+1} = \lim_{t \uparrow \infty} Q^{l+1}(t) > 0$. Exactly as before we see that there exists y_n^{l+1}, R_n^{l+1} such that (A.16)–(A.17) hold for $i \leqq l+1$, and $\sum_{i=1}^{l+1} \alpha_i \leqq 1$, $\alpha_{l+1} \leqq \alpha_l$, $|y_n^{i+1} - y_n^i| \xrightarrow[n]{} \infty$ for $i \leqq l$. By induction, we see that the only remaining case to be investigated is the case when the above construction yields sequences $(P_n^l)_l$, $(\alpha_l)_l$, $(y_n^l)_l$, $(R_n)_l$ such that (A.14)–(A.17) hold and

$$\alpha_{l+1} = \lim_{t \uparrow +\infty} \lim_n Q_n^{l+1}(t), \quad Q_n^{l+1}(t) = \operatorname*{Sup}_{y \in \mathbb{R}^l} P_n^{l+1}(B(y,t))$$

$$P_n^{l+1} = 1_{B(y_n^l, R_n^l)^c} P_n^l$$

for all $l \geqq 1$ (with $P_n^1 = P_n$). Because of (A.14) we see that $\alpha_l \xrightarrow[l]{} 0$. Now in order to prove (A.18) we argue by contradiction: assume (A.18) does not hold then (with our conventions) there exists $\alpha > 0$ such that

$$P_n(B(y_n, R) \cap A_n) \geqq \alpha, \quad \forall n \geqq 1$$

for some $y_n \in \mathbb{R}^k$, $R < \infty$. Next, choose l large enough so that $\alpha_l < \alpha$. Obviously,

$$Q_n^l(R) \geqq P_n^l(B(y_n, R)) \geqq P_n(B(y_n, R) \cap A_n) \geqq \alpha > \alpha_l,$$

and we reach a contradiction with the definition of α_l by taking the limit in n.

Lemma 2. *Let μ_n be a bounded sequence of bounded nonnegative measures on $\mathbb{R}^k$. Assume that $\underline{\lim}_n Q_n(t_0) > 0$ for some $t_0 > 0$, where $Q_n(t) = \sup_{y \in \mathbb{R}^k} \mu_n(B(y,t))$. Then there exists a subsequence that we still denote by μ_n for which the following holds: for all $t > 0$, $Q_n(t) \xrightarrow[n]{} Q(t)$ for some nondecreasing function Q and denoting by $\alpha = \lim_{t \uparrow \infty} Q(t)$, there exists $y_n \in \mathbb{R}^k$ such that*

$$\forall \varepsilon > 0, \quad \exists R < \infty, \quad \forall n \geqq 1, \quad \mu_n(B(y_n, R)) \geqq \alpha - \varepsilon. \tag{A.19}$$

Remark. It is easy to build $R_n \xrightarrow[n]{} \infty$ such that $Q_n(R_n) \xrightarrow[n]{} \alpha$, in which case (A.19) implies

$$\mu_n(B(y_n, R_n)) \xrightarrow[n]{} \alpha. \tag{A.20}$$

Proof of Lemma 2. Again, everything we say is correct modulo the extraction of enough subsequences. Let $\alpha_1 \in (0, \alpha)$, there exist R_1 and $y_n^1 \in \mathbb{R}^k$ such that $\mu_n(B(y_n^1, R_1)) \geqq \alpha_1$. With our conventions, we may assume that $\mu_n(B(y_n^1, t)) \xrightarrow[n]{} \bar{Q}^1(t)$ for all $t > 0$, where $\bar{Q}^1$ is nondecreasing, and let $\beta_1 = \lim_{t \uparrow \infty} Q^1(t)$. Clearly, $\beta_1 \in [\alpha_1, \alpha]$, and if $\beta_1 = \alpha$, we conclude. If $\beta_1 < \alpha$, we choose $\tilde{R}_n^1$ such that

$$\tilde{R}_n^1 \xrightarrow[n]{} \infty, \quad \mu_n(B(y_n^1, \tilde{R}_n^1)) \xrightarrow[n]{} \beta_1.$$

Then, let $R_n^1 \leqq \tilde{R}_n^1$, $\tilde{R}_n^1 \xrightarrow[n]{} \infty$, $\dfrac{R_n^1}{\tilde{R}_n^1} \xrightarrow[n]{} 0$; we still have

$$\mu_n(B(y_n^1, R_n^1)) \xrightarrow[n]{} \beta_1.$$

And we set $\mu_n^1 = \mu_n$, $\mu_n^2 = 1_{B(y_n^1, R_n^1)^c} \mu_n$. We may assume that the concentration function Q_n^2 of μ_n^2 converges for all $t > 0$ to some nondecreasing function Q^2. We claim that $\lim_{t\uparrow\infty} Q^2(t)=\alpha$. Indeed, for all $\varepsilon<\alpha-\beta_1$, there exist $R'<\infty$, $z_n\in\mathbb{R}^k$ such that

$$\mu_n(B(z_n,R'))\geqq\alpha-\varepsilon>\beta_1$$

Hence, $B(z_n,R')$ is not contained in $B(y_n^1,\tilde{R}_n^1)$, and thus for n large enough $B(z_n,R')\cap B(y_n^1,R_n^1)=\emptyset$. Therefore

$$\mu_n^2(B(z_n,R'))=\mu_n(B(z_n,R'))\geqq\alpha-\varepsilon,$$

and our claim is proved.

Then, we choose $y_n^2\in\mathbb{R}^k$, R_2 as we choose R_1 and y_n^1, and we may assume that $\mu_n^2(B(y_n^2,t))\underset{n}{\longrightarrow}\bar{Q}^2(t)$ for all $t>0$, where $\bar{Q}^2$ is nondecreasing, and we denote by $\beta_2=\lim_{t\uparrow\infty} Q^2(t)$. Again, $\beta_2\in[\alpha_1,\alpha]$. If $\beta_2=\alpha$, we conclude easily, while if $\beta_2<\alpha$ we choose $\tilde{R}_n^2$ and R_n^2 as above....

Repeating this argument and observing that as long as $\beta_l<\alpha$, we find

$$\mu_n^j(B(y_n^j,R_j))\geqq\alpha_1,\quad \text{for}\quad 1\leqq j\leqq l,$$

hence

$$\mu_n\left(\bigcup_{j=1}^{l} B(y_n^j,R_j)\right)=\bigcup_{j=1}^{l}\mu_n^j(B(y_n^j,R_j))\geqq l\alpha_1,$$

and we reach a contradiction for l large, proving the lemma.

Acknowledgements. The author would like to thank E.H. Lieb and B. Simon for suggesting the question treated here, A. Bahri for useful discussions and the referee for valuable suggestions.

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Communicated by B. Simon

Received March 20, 1986; in revised form September 23, 1986