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HARTREE-FOCK THEORY IN NUCLEAR PHYSICS (*)

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Abstract — *We present the Hartree-Fock approximation method for the many-body problems in Quantum Mechanics corresponding to the interaction of neutrons and protons We study the various forms of Hartree-Fock equations, the questions related to spin-dependence and spin-orbit forces, symmetries of the nucleus and symmetry breakings and time-dependent Hartree-Fock equations*

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I. INTRODUCTION

This paper is devoted to a general presentation of Hartree-Fock equations and related questions, and we will be mainly interested in the application of Hartree-Fock method to Nuclear Physics.

As it is well-known, the Hartree-Fock method was introduced by D. Hartree [23], V. Fock [17] and J. C. Slater [45] to approximate the ground state (and its energy) of general N-body problems in Quantum Physics. And the main application of this method was, in Atomic Physics, the study of Coulomb systems (atoms and molecules) with the purely Coulomb Hamiltonian of electrons interacting with static nucleii.

In Nuclear Physics, the use of Hartree-Fock methods to compute the ground state of nucleii is quite recent (see for example the review papers by H. Bethe [7], J. W. Negele [41], [42], P. Quentin and H. Flocard [44] and the references therein); among other reasons, this delay was due to the lack of understanding of strong interaction and thus to the difficulty of deriving realistic Hamiltonians to describe the *interaction of nucleons* (neutrons and protons). Let us immediately emphasize several important differences between the N-body Hamilto-

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nians arising in Atomic and Nuclear Physics

(i) *translation invariance* of the center of mass in Nuclear Physics (and no 1-body terms),

(ii) very different 2-body potentials (in Nuclear Physics the potentials have very *short range*),

(iii) large numbers of particles (nucleons)

We will come back on these differences and we will mention others such as the use of phenomenological density-dependent forces

From the mathematical viewpoint, these differences lead to equations (Hartree-Fock equations, HF in short) of a completely different nature And we do not know of any reference in the mathematical (or mathematical physics) literature dealing with HF equations in Nuclear Physics, while there are many references for HF equations (or at least Hartree equations) in Atomic Physics (see for example E H Lieb and B Simon [30], E H Lieb [29], P L Lions [32] and the references therein)

Our goal here is to present to mathematicians the basics of Hartree-Fock method (section II below) together with the known mathematical results on HF equations in the context of Nuclear Physics As we will see, many problems remain by large open and we present sometimes model, simplified problems which, hopefully, should preserve the same features than the exact HF systems of equations

We first describe the HF method (section II) which approximates a linear problem with a single unknown function in large dimensions by a non-linear one in 3 dimensions with a large number of unknown functions (the computational advantage being obvious) If one is interested in the ground state of a nucleus, the resulting problem by HF method is roughly speaking *a semi-linear vector valued minimization problem with constraints on* $\mathbb{R}^3$ *which is translation invariant* This is typical of problems which can be analyzed by the so-called *concentration-compactness method* (*cf* P L Lions [33], [34]) We explain in sections III-V the existence results we can obtain, adopting a layered presentation to cover more and more realistic problems (from the physics viewpoint) However, we do not consider in these sections the possibility of spin-dependence and spin-orbit forces until section VI

In section VII we go back to the original Hamiltonians and we discuss the various approximations including Thomas-Fermi classical approximation. Section VIII is devoted to the search of solutions of HF equations with symmetries while section IX is a very small contribution to the understanding of symmetry breakings of the nucleus In section X, we describe the external field method which is an important tool for the numerical computation of the ground state

Section XI is devoted to various considerations on time-dependent Hartree-Fock (TDHF in short) equations such as the *orbital stability* of the minima of HF problems and the study of other *periodic solutions*. From the mathematical viewpoint TDHF equations are systems of semilinear Schrödinger equations.

Finally, the last section (XII) concerns another approximation (somewhat related to the HF method) known as the Hartree-Fock-Bogolyubov method (HFB in short) and we refer to J. Dechargé and D. Gogny [14], J. G. Valatin [47], for the Physics background of this method.

There are important questions related to HF equations that we will not consider here namely the question of numerical analysis of HF equations, the RPA system and questions related to WKB approximations when $\hbar$ goes to 0. We hope to come back on these questions in future publications.

Let us finally mention that we will not assume any knowledge of Quantum Physics from the reader, but that we will try as much as possible to keep present the Physics motivations. The authors would like to thank Mr. R. Dautray for bringing HF theory in Nuclear Physics to the attention of the second author, and for stimulating their interdisciplinary collaboration.

II. PRESENTATION OF HARTREE-FOCK METHOD

The basic object we consider is a A-body Hamiltonian that we denote by H, where A is a positive integer : in Nuclear Physics, $A = N + Z$ with N number of neutrons and Z number of protons. The precise quantum system of A interacting nucleons is supposed to be described by the Hamiltonian H

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{A} \Delta_i + \sum_{i<j} V(x_i - x_j) \tag{1}$$

where V is a given potential (function on $\mathbb{R}^3$), $\hbar$ is the Planck constant, m is the mass of the nucleon (we neglect here as usual the small difference of mass between neutrons and protons) so $\frac{\hbar^2}{2m}$ may be thought of as a given positive constant. The points x_i $(1 \leqslant i \leqslant A)$ are generic points of $\mathbb{R}^3$ and the notation Δ_i means the Laplacian with respect to the group x_i of variables.

The Hamiltonian H is, at least formally, a self-adjoint operator acting on the closed subspace of $L^2((\mathbb{R}^3)^A)$ consisting of antisymmetric functions Φ of $x = (x_1, \ldots, x_A) \in (\mathbb{R}^3)^A$ i.e.

$$\Phi(x_{\sigma(1)}, \ldots, x_{\sigma(A)}) = (-1)^{|\sigma|}\,\Phi(x_1, \ldots, x_A) \tag{2}$$

for all $x_i \in \mathbb{R}^3$ $(1 \leqslant i \leqslant A)$ and for all permutations σ of $\{1, \ldots, A\}$ where $|\sigma|$

denotes the signature of σ. We denote by $\mathscr{H}$ this subspace. This important constraint (2) corresponds to the fundamental Pauli principle and is due to the fact that nucleons are fermions.

Before going further in the description of HF method, let us point out that, for physically correct Hamiltonians H, Φ should depend on spin and H should incorporate spin-orbit terms and a particular 3-body term. We deliberately ignore those terms in this section to keep the ideas clear even if in next section the last term equivalent to a density-dependent term is incorporated. Finally, we make no distinction between nucleons.

Of course, the interaction is mainly described by the choice of the potential V : let us mention some typical examples in Nuclear Physics

$$V(x) = \alpha\, e^{-\mu|x|^2} + \beta\, e^{-\nu|x|^2}, \qquad \alpha, \beta \in \mathbb{R}, \qquad \mu, \nu > 0 \tag{3}$$

or

$$V(x) = \alpha\, e^{-\mu|x|}(1/|x|) + \beta\, e^{-\nu|x|}(1/|x|), \qquad \alpha, \beta \in \mathbb{R}, \qquad \mu, \nu > 0 \tag{4}$$

or

$$V(x) = \alpha\delta_0 - \beta\,\Delta\delta_0, \qquad \alpha \in \mathbb{R}, \qquad \beta > 0. \tag{5}$$

All these choices (and there are many others) respect the fundamental character of strong interaction : short range and intense at short distances. Notice that V is spherically symmetric and this also is a general feature of the potentials V used in Nuclear Physics.

Observe also that $\mathscr{H}$, H are invariant by translation of the center of mass $\bar{x} = \frac{1}{A}\sum_{i=1}^{A} x_i$ i.e.

$$\text{If } \Phi \in \mathscr{H}, \quad \tau_h \Phi = \Phi(x_1 + h, x_2 + h, \dots, x_A + h) \in \mathscr{H} \quad \text{for all} \quad h \in \mathbb{R}^3 \tag{6}$$

$$\tau_h(H\Phi) = H(\tau_h \Phi). \tag{7}$$

Of course, one wants to know the spectrum of H and its eigenfunctions. In particular, a fundamental role is played by the bottom of the spectrum which is obviously given by

$$E = \operatorname{Inf}\left\{ (H\Phi, \Phi)_{L^2} / \Phi \in \mathscr{H}, \int_{\mathbb{R}^{3A}} |\Phi|^2\, dx = 1 \right\}. \tag{8}$$

This is the so-called ground state energy. We will write sometimes E^A to recall the dependence on the number A. Of course, the above notation is formal since $(H\Phi, \Phi)_{L^2}$ is not defined in general on $\mathscr{H}$ but on a subspace whose description depends on V : we will ignore those technicalities in this section. Let us finally mention that any minimum of (8) is called a ground state (in fact, we have made here so many simplifications that one can prove there exists no minimum of (8) because of the translation invariance — see section VII).

In Nuclear Physics, one has to deal with nucleii for which the number A of nucleons is large (up to 240) and this is why the direct computation of (8) is hopeless. Some approximation is needed. The original idea of D. Hartree [29] was to consider wave functions Φ (i.e. test functions Φ) of the form : $\Phi(x_1, \dots, x_A) = \prod_{i=1}^{A} \varphi_i(x_i)$. But clearly this choice contradicts the antisymmetry requirement (2). This led V. Fock [17] and J. C. Slater [45] to a better choice of Φ

$$\Phi(x_1, \dots, x_A) = \frac{1}{\sqrt{A\,!}} \sum_{\sigma} (-1)^{|\sigma|} \prod_{i=1}^{A} \varphi_{\sigma(i)}(x_i) = \frac{1}{\sqrt{A\,!}} \det(\varphi_i(x_j)) \tag{9}$$

where $\varphi_1, \dots, \varphi_A$ are A functions on $\mathbb{R}^3$ and the sum is over all permutations of $\{1, \dots, A\}$. Such a choice of Φ is called a Slater determinant.

Next, to check the normalization constraint of Φ in (8), we see that it is enough to impose

$$\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant A . \tag{10}$$

Indeed, we then have

$$\begin{aligned} \int_{\mathbb{R}^{3A}} |\Phi|^2 \, dx &= \frac{1}{A\,!} \sum_{\sigma,\sigma'} (-1)^{|\sigma|+|\sigma'|} \prod_i \int_{\mathbb{R}^3} \varphi_{\sigma(i)}(x_i) \, \varphi^*_{\sigma'(i)}(x_i) \, dx_i \\ &= \frac{1}{A\,!} \sum_{\sigma,\sigma'} (-1)^{|\sigma|+|\sigma'|} \prod_i \delta_{\sigma(i)\sigma'(i)} \\ &= \frac{1}{A\,!} \sum_{\sigma=\sigma'} (-1)^{|\sigma|+|\sigma'|} = 1 . \end{aligned}$$

Therefore, the HF approximation consists in replacing E in (8) by

$$E_{\mathrm{HF}} = \mathrm{Inf} \left\{ (H\Phi, \Phi)_{L^2} / \Phi = \det(\varphi_i(x_j)), \int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij} \right\} . \tag{11}$$

Observe that we have of course

$$E \leqslant E_{\mathrm{HF}} . \tag{12}$$

Next, it is possible to rewrite $(H\Phi, \Phi)_{L^2}$ quite simply when Φ is given by a Slater determinant. Indeed, we have for all $i < j$

$$\int_{\mathbb{R}^{3A}} |\nabla_i \Phi|^2 \, dx = \frac{1}{A\,!} \sum_{\sigma,\sigma'} (-1)^{|\sigma|+|\sigma'|} \left(\prod_{k \neq i} \int_{\mathbb{R}^3} \varphi_{\sigma(k)}(x_k)\, \varphi^*_{\sigma'(k)}(x_k)\, dx_k \right\} \times$$

$$\times \int_{\mathbb{R}^3} (\nabla \varphi_{\sigma(i)}(x_i), \nabla \varphi^*_{\sigma'(i)}(x_i))\, dx_i$$

$$= \frac{1}{A\,!} \sum_{\sigma,\sigma} (-1)^{|\sigma|+|\sigma'|} \left(\prod_{k \neq i} \delta_{\sigma(k)\sigma'(k)} \right) \times$$

$$\times \int_{\mathbb{R}^3} (\nabla \varphi_{\sigma(i)}(x_i), \nabla \varphi^*_{\sigma'(i)}(x_i))\, dx_i$$

$$= \frac{1}{A\,!} \sum_{\sigma} \int_{\mathbb{R}^3} |\nabla \varphi_{\sigma(i)}(x)|^2 \, dx$$

$$= \frac{1}{A} \sum_{i=1}^{A} \int_{\mathbb{R}^3} |\nabla \varphi_i(x)|^2 \, dx$$

while

$$\int_{\mathbb{R}^{3A}} V(x_i - x_j)\, |\Phi|^2 \, dx =$$

$$= \frac{1}{A\,!} \sum_{\sigma'\sigma'} (-1)^{|\sigma|+|\sigma'|} \left(\prod_{k \neq i,\, j} \int_{\mathbb{R}^3} \varphi_{\sigma(k)}(x_k)\, \varphi^*_{\sigma'(k)}(x_k)\, dx_k \right) \times$$

$$\times \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} V(x_i - x_j)\, \varphi_{\sigma(i)}(x_i)\, \varphi_{\sigma(j)}(x_j)\, \varphi^*_{\sigma'(i)}(x_i)\, \varphi^*_{\sigma'(j)}(x_j)\, dx_i\, dx_j =$$

$$= \frac{1}{A\,!} \sum_{\sigma} \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} |\varphi_{\sigma(i)}(x)|^2\, V(x-y)\, |\varphi_{\sigma(j)}(y)|^2 \, dx\, dy \, +$$

$$- \frac{1}{A\,!} \sum_{\sigma} \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} \varphi_{\sigma(i)}(x)\, \varphi^*_{\sigma(j)}(x)\, V(x-y)\, \varphi^*_{\sigma(i)}(y)\, \varphi_{\sigma(j)}(y)\, dx\, dy\,.$$

And we obtain the following expressions

$$E_{\mathrm{HF}} = \operatorname{Inf} \left\{ E(\varphi_1, \ldots, \varphi_A) / \varphi_i \in L^2(\mathbb{R}^3)\,, \quad \int_{\mathbb{R}^3} \varphi_i\, \varphi_j^* dx = \delta_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant A \right\} \tag{13}$$

with

$$E(\varphi_1, \ldots, \varphi_A) = \frac{\hbar^2}{2m} \sum_{i=1}^{A} \int_{\mathbb{R}^3} |\nabla \varphi_i|^2 \, dx + \\ + \sum_{i<j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |\varphi_i(x)|^2 V(x-y) |\varphi_j(y)|^2 \, dx \, dy \\ - \sum_{i<j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \varphi_i(x) \varphi_j^*(x) V(x-y) \varphi_i^*(y) \varphi_j(y) \, dx \, dy \quad (14)$$

or equivalently

$$E(\varphi_1, \ldots, \varphi_A) = \frac{\hbar^2}{2m} \sum_{i=1}^{A} \int_{\mathbb{R}^3} |\nabla \varphi_i|^2 \, dx + \\ + \frac{1}{2} \sum_{i,j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |\varphi_i(x)|^2 V(x-y) |\varphi_j(y)|^2 \, dx \, dy \\ - \frac{1}{2} \sum_{i,j} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \varphi_i(x) \varphi_j^*(x) V(x-y) \varphi_i^*(y) \varphi_j(y) \, dx \, dy . \quad (15)$$

The second term is often called the direct term while the third one is called the exchange term. We will also often denote by $\tau(x)$ the density of kinetic energy $\tau = \sum_{i=1}^{A} |\nabla \varphi_i(x)|^2$, $\rho(x)$ the density $\rho = \sum_{i=1}^{A} |\varphi_i(x)|^2$ and $\rho(x, y)$ the density matrix $\rho(x, y) = \sum_{i=1}^{A} \varphi_i(x) \varphi_i^*(y)$. Observe that we may simply write E as

$$E(\varphi_1, \ldots, \varphi_A) = \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} \tau \, dx + \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \rho(x) V(x-y) \rho(y) \, dx \, dy + \\ - \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} V(x-y) |\rho(x, y)|^2 \, dx \, dy . \quad (16)$$

The HF minimization problem (13) is nonlinear, nonconvex in general, with constraints and is invariant by translations (translating at the same time all φ_i), rotations in $\mathbb{R}^3$ and by unitary transforms of $(\varphi_1, \ldots, \varphi_A)$ in $\mathbb{C}^A$. In fact, in the examples given in next sections, the HF minimization problems will be slightly different (but still with the same general features) : an additional nonlinear term will be included in E corresponding to a 3-body term in H equivalent to a density-dependent 2-body term. We will come back on the realistic H being used in Nuclear Physics in section VII while we analyze in section IV-V

HF problems like (13) deduced from various examples of these realistic Hamiltonians by the method described above.

The Euler-Lagrange equations corresponding to the minimization problem (13) may be written as

$$-\frac{\hbar^2}{2m}\Delta\varphi_i + (\rho * V)\varphi_i - \int_{\mathbb{R}^3}\varphi_i(y)\left[\frac{1}{2}V(x-y) + \frac{1}{2}V(y-x)\right]\rho(x,y)\,dy =$$

$$= \sum_j e_{ij}\,\varphi_j \quad \text{in} \quad \mathbb{R}^3$$

for some hermitian matrix (e_{ij}) of Lagrange multipliers. Now, observe that if U is unitary and diagonalizes (e_{ij}) then $(\overline{\varphi}_1, \ldots, \overline{\varphi}_A) = U(\varphi_1, \ldots, \varphi_A)$ is still a minimum if $(\varphi_1, \ldots, \varphi_A)$ minimizes (13). And $(\overline{\varphi}_1, \ldots, \overline{\varphi}_A)$ now solves

$$-\frac{\hbar^2}{2m}\Delta\overline{\varphi}_i + (\rho * V)\,\overline{\varphi}_i - K\overline{\varphi}_i = e_i\,\overline{\varphi}_i \quad \text{in} \quad \mathbb{R}^3 \tag{17}$$

for some constant e_i, where K is the operator defined by

$$K\varphi(x) = \int_{\mathbb{R}^3}\varphi(y)\left[\frac{1}{2}V(x-y) + \frac{1}{2}V(x-y)\right]\rho(x,y)\,dy\,.$$

In particular, the constants $e_1, \ldots, e_A$ are eigenvalues of the operator $\left(-\frac{\hbar^2}{m}\Delta + (\rho * V) - K\right)$. Notice also that, at least in all the examples considered below, these eigenvalues $e_1, \ldots, e_A$ are non positive.

We conclude this section by a brief discussion of the validity of HF method : notice that it is an approximation of the " true " problem (8) and that, a priori, it gives only a bound from above of the ground state energy E (recall (12)). On the other hand, there are various reasons to use it and thus study it : first of all, it gives good numerical results and there are almost no substitutes to compute the ground state of E. A more " scientific " reason is its asymptotic validity as $A \to +\infty$ (for general V) as proved by E. H. Lieb and B. Simon [30], [31] : we will come back on this point in section VII.

III. A MODEL CASE

To give an idea of the type of HF problems which are encountered in Nuclear Physics, we will consider in this section a very simplified problem : we build a scalar problem ($A = 1$) with Skyrme's interaction as in D. Vautherin and D. M. Brink [48] skipping the spin dependence. In the next section, we will consider the general case of HF problems with Skyrme's interaction but without spin dependence. The functional (16) becomes in this case

$$E(\varphi) = \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx - \frac{\alpha}{4}\int_{\mathbb{R}^3} |\varphi|^4\,dx + \frac{\beta}{6}\int_{\mathbb{R}^3} |\varphi|^6\,dx + \\ + \frac{\gamma}{4}\int_{\mathbb{R}^3} |\varphi|^2\,|\nabla\varphi|^2\,dx + \frac{\delta}{16}\int_{\mathbb{R}^3} |\nabla|\varphi|^2|\,dx$$

where $\alpha, \beta, \gamma, \delta$ are constants such that : $\alpha > 0, \beta > 0, \gamma > 0, \gamma + \delta > 0$. This functional corresponds (essentially) to a potential V of the form (5) with the additional term $\left(\frac{\beta}{6}\int_{\mathbb{R}^3} |\varphi|^6\,dx\right)$.

Then the HF minimization problem becomes

$$I = \operatorname{Inf}\left\{ E(\varphi)/\varphi \in X\,,\ \int_{\mathbb{R}^3} |\varphi|^2\,dx = 1 \right\} \tag{19}$$

where the minimizing class X is defined by

$$X = \left\{ \varphi \in H^1(\mathbb{R}^3)\,(*)\,,\quad \int_{\mathbb{R}^3} |\varphi|^2\,|\nabla\varphi|^2\,dx < \infty \right\}.$$

Before stating our main existence result, let us recall that a minimizing sequence (φ_n) is a sequence (φ_n) in X satisfying

$$\int_{\mathbb{R}^3} |\varphi_n|^2\,dx = 1\,, \qquad E(\varphi_n) \underset{n}{\to} I\,.$$

We have the

THEOREM III.1 : *For every minimizing sequence $(\varphi_n)_n$ of the minimization problem* (19) *one can find y_n in $\mathbb{R}^3$ such that the new minimizing sequence $\varphi_n(\cdot + y_n)$ is relatively compact in $H^1(\mathbb{R}^3)$ if and only if $I < 0$. In particular, if $I < 0$ there exists a minimum of* (19). *In addition, $I < 0$ if and only if $\alpha > \alpha_0$ where α_0 is a positive constant depending on $\frac{\hbar^2}{m}$, β, γ, δ, which goes to 0 as $\frac{\hbar^2}{m}$ goes to 0. If $\alpha \leqslant \alpha_0$ there are minimizing sequences converging to 0 in $L^p(\mathbb{R}^3)$ for $2 < p \leqslant \infty$. Finally if $\alpha < \alpha_0$ there is no minimum of*(19).

(*) $H^1(\mathbb{R}^3) = \{ \psi \in L^2(\mathbb{R}^3), \nabla\psi\ L^2(\mathbb{R}^3) \}$.

Remarks : i) Further properties of minima of (19) are given below.

ii) Scalar problems like (19) have already been studied by several authors : we will only mention the works by W. Strauss [46], C. V. Coffman [13], H. Berestycki and P. L. Lions [5], P. L. Lions [40]. The methods in these works yield only the existence of a minimum if I < 0, using a symmetrization argument which is outlined in the proof of Proposition III.2 below and which no longer applies to more realistic problems such as the ones studied in the following sections.

iii) In fact it is possible to treat the case $\hbar = 0$: in that case every minimizing sequence in the class

$$\left\{ \varphi \in L^2(\mathbb{R}^3) ; (\operatorname{Re} \varphi)^2 , (\operatorname{Im} \varphi)^2 \in H^1(\mathbb{R}^3) ; \int_{\mathbb{R}^3} |\varphi|^2 |\nabla\varphi|^2 \, dx < \infty \right\}$$

is relatively compact say in L^2 up to a translation and there exists a minimum which is the limit of minima of (19) as $\hbar \to 0$. ■

Before proving Theorem III.1, we prove the

Proposition III.2 : *Assume that $I < 0$. Then there exists a minimum of* (19) *which is spherically symmetric, positive and decreasing with respect to* $r = |x|$.

Proof : In view of Theorem III.1, there exists a minimum φ of (19). Then considering the spherical nonincreasing rearrangement of $|\varphi|$, one checks easily that E is decreased and thus a minimum with the above properties is found. ■

We now turn to the

Proof of Theorem III.1 : We are going to apply the concentration-compactness arguments (cf. P. L. Lions [33]). Hence we introduce

$$I_\lambda = \operatorname{Inf}\left\{ E(\varphi)/\varphi \in X , \int_{\mathbb{R}^3} |\varphi|^2 \, dx = \lambda \right\} \tag{20}$$

where $\lambda > 0$. Then, applying the arguments of [33], we deduce that any minimizing sequence of (19) is relatively compact up to a translation if and only if I the following conditions holds

$$I_1 < I_\alpha + I_{1-\alpha}, \qquad \forall \alpha \in (0, 1). \tag{S.1}$$

We will not redo the proof in [33] but we will only make a few formal observations in order to explain the role of (S.1). The main difficulty in the above statement is the " if " part : in [33], it was proved that if a minimizing sequence is not relatively compact up to a translation then roughly speaking it breaks at least into two parts which are essentially supported in two disjoint closed sets whose distance goes to ∞. Let us denote those two parts by φ_n^1, φ_n^2 so $\varphi_n \simeq \varphi_n^1 + \varphi_n^2$; we may assume that $\int_{\mathbb{R}^3} (\varphi_n^1)^2 \, dx \underset{n}{\to} \alpha$, $\int_{\mathbb{R}^3} (\varphi_n^2)^2 \, dx \underset{n}{\to} 1 - \alpha$. The above dichotomy then yields

$$I = \lim_n E[\varphi_n] \geqslant \varliminf_n E[\varphi_n^1] + \varliminf_n E[\varphi_n^2] \geqslant I_\alpha + I_{1-\alpha}$$

and if (S.1) holds this is not possible.

The arguments of [33] apply : the only modification consists in checking that if φ_n is bounded in $H^1(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} |\varphi_n|^2 |\nabla\varphi_n|^2 \, dx \leqslant c$ (indep. of n) and φ_n converges weakly in H^1 to some φ then

$$\varliminf_n \frac{\gamma}{4} \int_{\mathbb{R}^3} |\varphi_n|^2 |\nabla\varphi_n|^2 \, dx + \frac{\delta}{16} \int_{\mathbb{R}^3} |\nabla |\varphi_n|^2|^2 \, dx \geqslant$$
$$\geqslant \frac{\gamma}{4} \int_{\mathbb{R}^3} |\varphi|^2 |\nabla\varphi|^2 \, dx + \frac{\delta}{16} \int_{\mathbb{R}^3} |\nabla |\varphi|^2|^2 \, dx \, .$$

The proof of this claim is a simple consequence of Lemma III.3, which is stated and proved after the proof of Theorem III.1.

We next show that (S.1) is equivalent to $I < 0$ and that one has always $I_\lambda \leqslant 0$: indeed, let $\varphi \in \mathcal{D}(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} |\varphi|^2 \, dx = \lambda$ and let $\varphi_\sigma(x) = \sigma^{-3/2} \varphi\left(\frac{x}{\sigma}\right)$ for $\sigma > 0$. Obviously

$$I_\lambda \leqslant E[\varphi_\sigma] = \frac{1}{\sigma^2} \left\{ \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} |\nabla\varphi|^2 \, dx \right\} +$$
$$- \frac{1}{\sigma^3} \left\{ \frac{\alpha}{4} \int_{\mathbb{R}^3} |\varphi|^4 \, dx \right\} + \frac{1}{\sigma^6} \left\{ \frac{\beta}{6} \int_{\mathbb{R}^3} |\varphi|^6 \, dx \right\} +$$
$$+ \frac{1}{\sigma^5} \left\{ \frac{\gamma}{4} \int_{\mathbb{R}^3} |\varphi|^2 |\nabla\varphi|^2 \, dx + \frac{\delta}{16} \int_{\mathbb{R}^3} |\nabla |\varphi|^2|^2 \, dx \right\}$$

and letting $\sigma \to +\infty$, we prove that $I_\lambda \leqslant 0$. Next, by a similar scaling argument we see for all $\theta > 1$, $\lambda > 0$

$$I_{\theta\lambda} = \operatorname{Inf}\left\{ \theta^{1/3}\left[\frac{\hbar^2}{2\,m}\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx\right] + \right.$$
$$+ \theta\left[-\frac{\alpha}{4}\int_{\mathbb{R}^3}|\varphi|^4\,dx + \frac{\beta}{6}\int_{\mathbb{R}^3}|\varphi|^6\,dx\right] +$$
$$+ \theta^{1/3}\left[\frac{\gamma}{4}\int_{\mathbb{R}^3}|\varphi|^2\,|\nabla\varphi|^2\,dx + \frac{\delta}{16}\int_{\mathbb{R}^3}|\nabla|\varphi|^2|^2\,dx\right]\Big/\ \varphi\in X\,,$$
$$\left.\int_{\mathbb{R}^3}|\varphi|^2\,dx = \lambda\right\}.$$

Now we claim that if $I_\lambda < 0$ the infimum in I_λ may be restricted to those φ satisfying

$$A(\varphi) = \frac{\hbar^2}{2\,m}\int_{\mathbb{R}^3}|\nabla\varphi|^2\,dx + \frac{\gamma}{4}\int_{\mathbb{R}^3}|\varphi|^2\,|\nabla\varphi|^2\,dx +$$
$$+ \frac{\delta}{16}\int_{\mathbb{R}^3}|\nabla|\varphi|^2|^2\,dx \geqslant \nu$$

for some $\nu > 0$. Indeed if there were a minimizing sequence of I_λ such that $A(\varphi_n) \underset{n}{\to} 0$, then by Sobolev embeddings $\varphi_n \underset{n}{\to} 0$ in $L^p(\mathbb{R}^3)$ for $2 < p \leqslant 6$ (in fact $p \leqslant 12$ here) and so $\int|\varphi_n|^4\,dx \underset{n}{\to} 0$. But this means that $I_\lambda \geqslant 0$ and our claim is proved. Hence, we deduce

$$I_{\theta\lambda} < \theta\operatorname{Inf}\left\{E(\varphi)/\varphi\in X\,,\quad A(\varphi)\geqslant\nu\,,\quad \int_{\mathbb{R}^3}|\varphi|^2\,dx = \lambda\right\} = \theta I_\lambda$$

and this inequality holds if $I_\lambda < 0$. Then, a straightforward argument proves that (S.1) is equivalent to $I < 0$.

Observe also that the above scaling argument shows that if $I = 0$, there is a minimizing sequence (namely φ_σ as $\sigma \to +\infty$) which converges to 0 in L^p for $2 < p \leqslant \infty$.

We next discuss the inequality $I < 0$. It is obvious that $I < 0$ for α large enough. So let us denote by $\alpha_0 = \alpha_0\left(\frac{\hbar^2}{m}, \beta, \gamma, \delta\right)$ the least positive constant such that $I < 0$ for $\alpha > \alpha_0$ (observe that I is nonincreasing with respect to α). We have to prove that $\alpha_0 > 0$ or in other words that $I = 0$ for α small enough.

But using Sobolev and Hölder inequalities we find for $\varphi \in X$, $\int_{\mathbb{R}^3} |\varphi|^2 = 1$

$$E(\varphi) \geqslant c_0 \frac{\hbar^2}{2m}\left(\int_{\mathbb{R}^3} |\varphi|^6 \, dx\right)^{1/3} - \frac{\alpha}{4}\left(\int_{\mathbb{R}^3} |\varphi|^6 \, dx\right)^{1/2} + \frac{\beta}{6}\left(\int_{\mathbb{R}^3} |\varphi|^6 \, dx\right).$$

A simple study of the function of one real variable $c_0 \frac{\hbar^2}{2m} t^{1/3} - \frac{\alpha}{4} t^{1/2} + \frac{\beta}{6} t$ proves that $I = 0$ for α small enough.

The fact that α_0 goes to 0 as $\frac{\hbar^2}{m} \to 0$ can be seen from the expression of $E[\varphi_\sigma]$ given above.

Finally let $\bar{\alpha} < \alpha_0$, if there exists a minimum of I for $\bar{\alpha}$ we can test the minimization problem (19) for $\bar{\alpha} < \alpha \leqslant \alpha_0$ with this minimum and this gives a negative value for I contradicting the definition of α_0. ■

LEMMA III.3 : *Let $f_n \geqslant 0$ converge in L^1 to some $f \geqslant 0$, let g_n converge weakly in L^2 to some g. Then $f|g|^2 \in L^1$ and we have*

$$\varliminf_n \int f_n |g_n|^2 \geqslant \int f |g|^2 .$$

Proof : Let $M, R \in (0, \infty)$. We introduce a symmetric convex function Φ_R satisfying $0 \leqslant \Phi_R(z) \leqslant |z|^2$, $\Phi_R(z) = |z|^2$ for $|z| \leqslant R$, Φ_R is Lipschitz. It is clearly enough to prove that we have

$$\varliminf_n \int f_n |g_n|^2 \geqslant \int_{(f \leqslant M)} f \Phi_R(g) .$$

In order to do so we first observe that, without loss of generality, we may assume that $\Phi_R(g_n)$ converges weakly in L^2 to some h which satisfies $h \geqslant \Phi_R(g)$.

Next, we remark that we can conclude if we prove that

$$\int_{(f \leqslant M)} (f - f_n)^+ \, \Phi_R(g_n) \underset{n}{\to} 0 .$$

But this integral is easily bounded for all $\delta > 0$ by

$$\begin{aligned}\delta \int \Phi_R(g_n) + M \int_{(f - f_n \geqslant \delta)} \Phi_R(g_n) &\leqslant \delta \int | g_n |^2 + C(M, R) \int_{(f - f_n \geqslant \delta)} | g_n | \\ &\leqslant C\delta + C(M, R) \{ \operatorname{meas}(f - f_n \geqslant \delta) \}^{1/2} \\ &\leqslant C\delta + C(M, R)\, \delta^{-1/2} \int | f - f_n |\end{aligned}$$

and we may conclude. ■

IV. SKYRME'S INTERACTION WITHOUT SPIN

In all this section we will consider only the so-called Skyrme's interaction thus following the approach by D. Vautherin and D. M. Brink [46]. To simplify the presentation we skip the spin dependence and we refer to section VI for the complete problems.

We begin this section by a special case which corresponds to the simplified situation where no differences are made between neutrons and protons ($N = Z$, no Coulomb interaction between protons). In fact, if isospin is " fixed " for neutrons and protons at the level of the original A-body problem, one can allow in the Slater determinant wave-functions which depend on the isospin and then one is also led to problems of the following form. In those cases the functional (16) becomes

$$E(\varphi_1, \ldots, \varphi_A) = \int_{\mathbb{R}^3} \frac{\hbar^2}{2m} \tau - \frac{\alpha}{4} \rho^2 + \frac{\beta}{4} \rho\tau + \frac{\gamma}{16} | \nabla\rho |^2 + \frac{\delta}{6} \rho^3 \, dx \quad (21)$$

where $\tau = \sum_{i=1}^{A} | \nabla\varphi_i |^2$, $\rho = \sum_{i=1}^{A} | \varphi_i |^2$. The constants $\alpha, \beta, \gamma, \delta$ satisfy

$$\alpha > 0, \qquad \beta > 0, \qquad \delta > 0, \qquad \beta + \gamma > 0. \quad (22)$$

As in the preceding section, only the last term $\frac{\delta}{6} \int_{\mathbb{R}^3} \rho^3 \, dx$ is not an obvious consequence of the HF method as described in section II : indeed this term (and analogous terms in this section and in the next one) comes from a 3-body term which is equivalent to a 2-body density dependent term in the Hamiltonian H. We will come back on this point in section VII.

The HF minimization problem may then be written as

$$I = \operatorname{Inf}\left\{ E(\varphi_1, \ldots, \varphi_A)/\varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho\tau \, dx < \infty, \right.$$
$$\left. \int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant A \right\}. \quad (23)$$

Before stating our main result on (23), we need to introduce a few notations : let $M = (m_{ij})$ be a nonnegative hermitian matrix, we introduce the following minimization problem

$$I_M = \operatorname{Inf}\left\{ E(\varphi_1, \ldots, \varphi_A)/\varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho\tau \, dx < \infty, \right.$$
$$\left. \int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = m_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant A \right\}. \quad (24)$$

Then, we observe that since E is invariant under unitary transforms of $(\varphi_1, \ldots, \varphi_A)$ then for any unitary matrix U in C^A

$$I_M = I_{U^{-1}MU} \quad (25)$$

so we may choose U so that $U^{-1} MU$ is diagonal and if $(m_1, \ldots, m_A)$ are the eigenvalues of M, $M_0 = \operatorname{diag}(m_1, \ldots, m_A)$ is the diagonal matrix with $(m_1, \ldots, m_A)$ as diagonal entries then $I_M = I_{M_0}$ and we will denote $I_M = I_{M_0} = I(m_1, \ldots, m_A)$. With these notations, $I = I_{\mathbb{1}} = I(1, \ldots, 1)$ where $\mathbb{1} = (\delta_{ij})$.

Finally, we will say that a sequence $(\varphi_1^n, \ldots, \varphi_A^n)$ in the minimizing set is relatively compact up to a translation if there exists y^n in $\mathbb{R}^3$ such that $(\tilde{\varphi}_1^n, \ldots, \tilde{\varphi}_A^n) = (\varphi_1^n(\cdot + y^n), \ldots, \varphi_A^n(\cdot + y^n))$ — which is still a sequence in the minimizing set — is relatively compact in H^1 and $|\nabla\tilde{\rho}^n|^2$, $\tilde{\rho}^n \tilde{\tau}^n$ are compact in L^1 (with obvious notations).

THEOREM IV.1 : i) *The infimum* $I \in (-\infty, 0]$ *and for all* $R < \infty$ *there exists* $C_R < \infty$ *such that* $\int_{\mathbb{R}^3} \rho + \tau + \rho\tau \, dx \leqslant C_R$ *if* $E(\varphi_1, \ldots, \varphi_A) \leqslant R$,

$$\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij} \, (\forall i, j), \int_{\mathbb{R}^3} \rho\tau \, dx < \infty .$$

ii) *Every minimizing sequence of the problem* (24) *is relatively compact up to a* *translation if and only if the following conditions holds*

$$I < I(m_1, ..., m_A) + I(1 - m_1, ..., 1 - m_A) \quad \text{for all} \quad (m_1, ..., m_A) \qquad (26)$$

such that $0 \leqslant m_i \leqslant 1$ *for* $1 \leqslant i \leqslant A$, $0 < \sum_i m_i < A$. *Of course, if* (26) *holds then there is a minimum of* (23).

iii) *If* $\alpha < \alpha_0$ *where* α_0 *is some positive constant depending on* $A, \frac{\hbar^2}{m}, \beta, \gamma, \delta$; *then* $I = 0$ *and there is no minimum of* (23).

Remarks : i) In general, we do not know how to check (26). The answer seems to be highly dependent on A in view of the numerical computations which have been performed. In any case, checking conditions (26) for numerical computations of ground states appears to be a good test since (26) means a certain stability of the absolute minimum.

ii) In fact, as seen below from the proof which again relies on the concentration-compactness arguments [33], the concentration-compactness method not only shows the necessity and sufficiency of (26) but also predicts what can happen on minimizing sequences. Let us give a few examples :

1) Suppose $I = 0$, then there are minimizing sequences converging to 0 in L^p for $p > 2$ and the density vanishes (in the sense of [33]).

2) Suppose (to simplify) that there exists a unique set of values $(\overline{m}_1, ..., \overline{m}_A)$ such that $0 \leqslant \overline{m}_i \leqslant 1$ for $1 \leqslant i \leqslant A$, $0 < \sum_i \overline{m}_i < A$, $I = I(\overline{m}_1, ..., \overline{m}_A) + I(1 - \overline{m}_1, ..., 1 - \overline{m}_A)$ while (26) holds for all $(m_1, ..., m_A) \neq (\overline{m}_1, ..., \overline{m}_A)$. In fact, this over simplification implies $\overline{m}_1 = \cdots = \overline{m}_A$ but we will ignore this for the sake of the argument. Two cases may occur : the simplest one is when the two minimization problems $I(\overline{m}_1, ..., \overline{m}_A)$, $I(1 - \overline{m}_1, ..., 1 - \overline{m}_A)$ satisfy the analogues of the subadditivity conditions (26). Then, there are minimizing sequences of (23) which are not relatively compact up to a translation and any such sequence $(\varphi_1^n, ..., \varphi_A^n)$ breaks in two parts :

$$\varphi_i^n = \psi_i^n + \chi_i^n, \qquad 1 \leqslant i \leqslant A$$

where ψ_i^n, χ_i^n are relatively compact up to a translation and are minimizing sequences of $I(\overline{m}_1, ..., \overline{m}_A)$, $I(1 - \overline{m}_1, ..., 1 - \overline{m}_A)$ and thus (extracting subsequences if necessary) converge to minima of these problems. In addition, roughly speaking, the distance between the supports of $\sum_i |\psi_i^n|^2$ and $\sum_i |\chi_i^n|^2$ goes to ∞ as $n \to \infty$. The second case concerns the situation when $I(\overline{m}_1, ..., \overline{m}_A)$ (or $I(1 - \overline{m}_1, ..., 1 - \overline{m}_A)$) does not satisfy the analogue of (26) : then we may continue the above argument and in turn ψ_i^n can break into two pieces. If we knew completely the function $I(m_1, ..., m_A)$, it would be possible to determine completely the behavior of minimizing sequences : vanishing, dichotomy into n parts converging to minima of subproblems, dichotomy into n parts with $(n - 1)$ pieces converging to minima of subproblems and one piece vanishing.

iii) Again, we can treat as well the case $\hbar = 0$ and the analogue of i) holds. ■

At this stage, it is interesting to briefly explain how all the above phenomena are related to various physical situations which essentially depend on the set (N, Z) caracterizing the numbers of neutrons and protons. In fact, it is experimentally observed that the existence of a nucleus crucially depends on the set (N, Z) as we explain now with the help of Figure 1 below taken from M. Effer [15]. In the plane (N, Z) the stable nuclei (infinite life-time) are indicated in black. Admitting that the A-body Hamiltonian and the Hartree-Fock approximation correctly represent the reality, these values of (N, Z) would correspond to " nice " minima in the problems we are considering here and below (the strict subadditivity inequalities should hold for such values). The dotted grey zone corresponds to unstable nuclei which are known today and whose lifetime may vary in between 10^{15} years and some milli-seconds. Let us mention that a little more than 2 000 nuclei are known : about 300 exist in nature while 1 900 were " built ". Between 2 000 and 4 000 additional nuclei are expected to exist (mostly unstable). Finally the majority of nuclei currently observed in nature (263 out of 287) are stable. The white zone, delimited by two lines, correspond to (unstable) nuclei which are to be discovered. For HF problems, those unstable nuclei correspond to minimization problems where the strict subadditivity inequalities do not hold and minimizing sequences break into several " compact " pieces (see a precise example below). The two lines, the so-called " drip-lines ", beyond which no nuclei are expected to exist, are precisely associated with the loss of exactly one neutron ($S_n = 0$) or one proton ($S_p = 0$). In our context, this situation would correspond to the case when $(\overline{m}_1, \dots, \overline{m}_A) = (1, 0, \dots, 0)$ in Remark ii) above i.e. minimizing sequences break into two parts : one which is " compact " and converges up to a translation to the minimum of a $I(0, 1, \dots, 1)$ while the other part vanishes. The zone beyond the drip lines should correspond to similar phenomena where minimizing sequences break into several pieces one of which vanishes.

In order to illustrate the situation concerning the unstable nuclei we shall restrict ourselves to two examples. The first one concerns the nucleus ${}^{144}_{60}\mathrm{Nd}$ $(Z = 60,\ N = 84)$ whose lifetime is quite long (about 2×10^5 years). This nucleus is unstable and eventually decays, emitting an alpha particle (elementary nucleus composed of 2 neutrons and 2 protons), into the two stable subsystems ${}^{140}_{58}\mathrm{Xe}$ and α and one writes

$${}^{144}_{60}\mathrm{Nd} \rightarrow {}^{140}_{58}\mathrm{Xe} + \alpha .$$

The other example is provided by the nucleus ${}^{240}_{94}\mathrm{Pu}$ which spontaneously fissions into two stable nuclei

$${}^{240}_{94}\mathrm{Pu} \rightarrow {}^{134}_{52}\mathrm{Te} + {}^{106}_{42}\mathrm{Mo}\,.$$

In our context (once more admitting the models are good enough to reproduce these fissions and this seems to be the case in view of HF numerical computations) this obviously corresponds to minimizing sequences breaking into two parts which converge (up to translations) to minima of appropriate subproblems. In fact, if we were to use a nuclear force realistic enough and if we knew completely the functions $I(m_1, \dots, m_A)$ we would be able to predict all unstability patterns (or confirm the numerical computations at least...).

We wish to conclude these physical considerations by indicating that HF minimization problems (with possibly the extension to HFB problems — see section XII) lead to numerical computations which reproduce quite well at least parts of the diagram below (stable nuclei, some unstable ones, drip lines...) : the restriction being essentially due to the difficulty of solving numerically these problems. And we refer to J. F. Berger, M. Girod and D. Gogny [6], M. Girod and B. Grammaticos [21], D. Vautherin and D. M. Brink [48], P. Quentin and H. Flocard [44], J. Negele [41], [42] (and the references given therein) for various extensive computations. Another observation consists in remarking that for unstable nuclei in fact several different fragmentations are often possible with one being more probable (statistically) and these various choices could be related to dichotomies of minimizing sequences corresponding to values of $\bar{m}_1, \dots, \bar{m}_A$ strictly between 0 and 1. Finally, we wish to warn the interested reader that the above considerations indicate that strict subadditivity inequalities may be very hard to check and in addition should depend in a sensitive way on A (or (N, Z) for problems below...).

Proof of Theorem IV.1 : It is enough to prove the existence of C_R. Remark that

$$\frac{\beta}{4}\rho\tau + \frac{\gamma}{16}|\nabla\rho|^2 = \frac{\beta}{4}\rho\tau + \frac{\gamma}{4}\left|\sum_i \mathrm{Re}(\varphi_i\,\nabla\varphi_i^*)\right|^2 \geqslant \frac{\beta+\gamma}{4}\rho\tau \geqslant 0$$

and $\frac{\alpha}{4}\rho^2 \leqslant \frac{\delta}{6}\rho^3 + C(\alpha, \delta)$ so

$$E(\varphi_1, \dots, \varphi_A) \geqslant \int_{\mathbb{R}^3} \frac{\hbar^2}{2m}\tau + \left(\frac{\beta+\gamma}{4}\right)\rho\tau\, dx - C(\alpha, \delta)$$

and i) is easily deduced. Again part ii) of the above result is a direct application

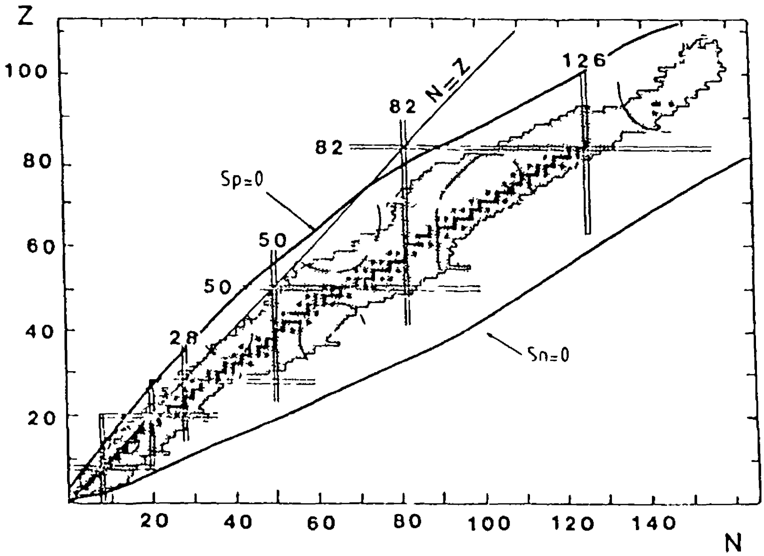

Fig. 1

of the concentration-compactness argument ([33]). We will not give the proof but instead we will explain the main idea used to prove the sufficiency of (26). If $(\varphi_1^n, ..., \varphi_A^n)$ is a minimizing sequence of (23), then we apply the lemma below (proved in [33]) with the probability P_n on $\mathbb{R}^3$ whose density is $\frac{1}{A}\rho^n$ (i.e. the density in Nuclear Physics terminology !).

LEMMA IV.1 : *Let $(P_n)_n$ be a sequence of probability measures on $\mathbb{R}^N$.*

Then there exists a subsequence that we still denote by P_n such that one of the following properties hold :

i) (compactness up to a translation) $\exists y^n \in \mathbb{R}^n, \forall \varepsilon > 0, \exists R < \infty$

$$P_n(B(y^n, R)) \geqslant 1 - \varepsilon .$$

ii) (vanishing) $\forall R < \infty, \ \operatorname*{Sup}_{y \in \mathbb{R}^N} P_n(B(y, R)) \underset{n}{\to} 0.$

iii) (dichotomy) $\exists \alpha \in (0, 1), \forall \varepsilon > 0, \forall M < \infty, \exists R_0 \geqslant M, \exists y_n \in \mathbb{R}^N, \exists R_n \underset{n}{\to} \infty$ such that

$$| P_n(B(y_n, R_0)) - \alpha | \leqslant \varepsilon , \quad | P_n(B(y_n, R_n)^c) - (1 - \alpha) | \leqslant \varepsilon . \quad \blacksquare$$

If P_n or ρ_n vanishes (case ii)) then (see [33]) $\varphi_n^1, ..., \varphi_n^A$ converge strongly in $L^p(\mathbb{R}^3)$ to 0 for $2 < p < 6$ (actually < 12) and thus $I = \lim_n E(\varphi_n^1, ..., \varphi_n^A) \geqslant 0$.

Since one checks easily by a scaling argument as in the proof of Theorem III.1 that $I_M \leqslant 0$, this means $I = 0$ and it contradicts (26).

If dichotomy occurs (case iii)) then we translate $(\varphi_n^1, \ldots, \varphi_n^A)$ by y^n and roughly speaking we split these functions into their " restrictions " to $B(y^n, R_0)$ and to $B(y^n, R_n)^c$ and we denote by $(\psi_n^1, \ldots, \psi_n^A)$, $(\chi_n^1, \ldots, \chi_n^A)$ the two parts. We may assume that

$$\int_{\mathbb{R}^3} \psi_n^i \psi_n^{j*} \, dx \underset{n}{\rightarrow} m_{ij}\,, \qquad \int_{\mathbb{R}^3} \chi_n^i \chi_n^{j*} \, dx \underset{n}{\rightarrow} \delta_{ij} - m_{ij}$$

for some hermitian matrix (m_{ij}) such that (essentially) $\sum_i m_{ii} = \alpha A$. The contradiction with (26) is obtained by remarking that

$$I = \lim_n E(\varphi_n^1, \ldots, \varphi_n^\alpha) \geqslant \underline{\lim}_n E(\psi_n^1, \ldots, \psi_n^A) + \underline{\lim}_n E(\chi_n^1, \ldots, \chi_n^A)$$
$$\geqslant I_M + I_{1-M}\,.$$

Therefore, if (26) holds then automatically we are in case i) and we conclude as in [33] provided one observes that since γ is not assumed to be positive there is a little difficulty to pass to the limit which is solved by the

LEMMA IV.2 : *Let $\varphi_n^1, \ldots, \varphi_n^A$ converge weakly in $H^1(\mathbb{R}^3)$ to $\varphi^1, \ldots, \varphi^A$. Assume in addition that $\rho_n \tau_n$ is bounded in $L^1(\mathbb{R}^3)$. Then $\rho\tau \in L^1(\mathbb{R}^3)$ and*

$$\begin{aligned} &\underline{\lim}_n \int_{\mathbb{R}^3} \rho_n \tau_n \, dx \geqslant \int_{\mathbb{R}^3} \rho\tau \, dx\,, \\ &\underline{\lim}_n \int_{\mathbb{R}^3} \rho_n \tau_n - \frac{1}{4} |\nabla \rho_n|^2 \, dx \geqslant \int_{\mathbb{R}^3} \rho\tau - \frac{1}{4} |\nabla \rho|^2 \, dx\,. \end{aligned} \tag{27}$$

Proof : The first part of (27) is a consequence of Lemma III.3. The second part will also be after a few considerations. We introduce the nonnegative, convex, quadratic functional for all $z \in C^A$, $\phi = (\varphi_1, \ldots, \varphi_A)$

$$Q(z, \nabla\phi) = \frac{|z|^2}{(1 + |z|^2)} \left(\sum_i |\nabla \varphi_i|^2 \right) - \frac{1}{(1 + |z|^2)} \left| \sum_i \mathrm{Re}\,(z_i \nabla \varphi_i^*) \right|^2 .$$

Observe that $Q(\phi, \nabla\phi) = (1 + \rho)^{-1} \left[\rho\tau - \frac{1}{4} |\nabla\rho|^2 \right]$.

Now, if we set $\phi_n = (\varphi_n^1, \ldots, \varphi_n^A)$, $g_n = \{ Q(\phi_n, \nabla\phi_n) \}^{1/2}$, g_n is bounded in $L^2(\mathbb{R}^3)$. And we may assume that g_n converges weakly in L^2 to some g. If we show that $g \geqslant \{ Q(\phi, \nabla\phi) \}^{1/2}$ where $\phi = (\varphi^1, \ldots, \varphi^A)$, then applying Lemma

III.3 with $f_n = (1 + \rho_n)$ we conclude easily showing the second half of (27) on any bounded domain of $\mathbb{R}^3$ $\left(\text{this is enough since } \rho\tau - \frac{1}{4}|\nabla\rho|^2 \geqslant 0\right)$.

Since $Q(z, \nabla\phi)^{1/2}$ is convex for all z, it is clearly enough to show that for any $\psi \in \mathscr{D}(\mathbb{R}^3)$

$$\int_{\mathbb{R}^3} \psi \,|\, Q^{1/2}(\phi_n, \nabla\phi_n) - Q^{1/2}(\phi, \nabla\phi_n) \,|\, dx \underset{n}{\to} 0 .$$

Since $Q^{1/2}$ is continuous on bounded sets, we introduce the local modulus

$$\omega_R(\delta) = \sup \{ \,|\, Q^{1/2}(z, p) - Q^{1/2}(z + h, p) \,|/|\, p \,| \leqslant R \,, |\, z \,| \leqslant R \,, |\, h \,| \leqslant \delta \,\}$$
$$\text{for all} \quad \delta > 0 \,, \quad R < \infty$$

and we split the above integral into integrals over several sets that we bound as follows :

- On $\{ \,|\, \nabla\phi_n \,| \geqslant R$ or $|\, \phi_n \,| \geqslant R$ or $|\, \phi \,| \geqslant R \,\}$, the integral is bounded by

$$C \int_{(-)} \psi(|\, \nabla\phi_n \,| + |\, \nabla\phi \,|)\, dx \leqslant C(\psi) \operatorname{meas}(-)^{1/2} \leqslant \frac{C(\psi)}{R} .$$

- On $\{ \,|\, \nabla\phi_n \,|, |\, \phi_n \,|, |\, \phi \,| \leqslant R ; |\, \phi_n - \phi \,| > \delta \,\}$, the integral is bounded by

$$C \int_{(|\phi_n - \phi| > \delta)} \psi(|\, \nabla\phi_n \,| + |\, \nabla\phi \,|)\, dx \leqslant C(\psi) \operatorname{meas}(|\, \phi_n - \phi) \,| > \delta)^{1/2} \underset{n}{\to} 0 .$$

- On $\{ \,|\, \nabla\phi_n \,|, |\, \phi_n \,|, |\, \phi \,| \leqslant R ; |\, \phi_n - \phi \,| \leqslant \delta \,\}$, the integral is bounded by

$$\omega_R(\delta) \int_{\mathbb{R}^3} \psi \, dx = C\omega_R(\delta) .$$

This enables us to conclude easily.

Another possible proof (communicated to us by H. Brézis) is the following : since $\rho_n \tau_n - \frac{1}{4}|\nabla\rho_n|^2$, $\rho\tau - \frac{1}{4}|\nabla\rho|^2$ are nonnegative, it is enough to show that for all M

$$\varliminf_n \int_{\bigcap_{i=1}^{A} (|\varphi^i| \leqslant M)} \rho_n \tau_n - \frac{1}{4}|\nabla\rho_n|^2 dx \geqslant \int_{\bigcap_{i=1}^{A} (|\varphi^i| \leqslant M)} \rho\tau - \frac{1}{4}|\nabla\rho|^2 \, dx .$$

Now, by Egorov's theorem, for all $\varepsilon > 0$ there exists a set E such that its complement has measure less than ε and φ_n^i converges uniformly to φ^i on E

for all i. Denoting by $F = E \cap \left(\bigcap_{i=1}^{A} (|\varphi^i| \leqslant M) \right)$, it is enough to show that

$$\underline{\lim}_n \int_F \rho_n \tau_n - \frac{1}{4} |\nabla \rho_n|^2 \, dx \geqslant \int_F \rho\tau - \frac{1}{4} |\nabla \rho|^2 \, dx .$$

Observe now that ρ_n, φ_n^i (for $1 \leqslant i \leqslant A$) are uniformly bounded on F and converge uniformly to ρ, φ^i. Therefore, we just have to prove

$$\underline{\lim}_n \int_F Q(\phi, \nabla\phi_n) \, dx \geqslant \int_F Q(\phi, \nabla\phi) \, dx .$$

To this end, we write $\phi_n = \phi + \psi_n$ and we obtain

$$Q(\phi, \nabla\phi_n) = Q(\phi, \nabla\phi) + Q(\phi, \nabla\psi_n) + 2\, Q(\phi, \nabla\phi, \nabla\psi_n)$$

where $Q(z, ., .)$ is the symmetric bilinear form associated with $Q(z, .)$.

To conclude, one just observes that $Q(\phi, \nabla\psi_n) \geqslant 0$, while by the weak convergence of $\nabla\psi_n$ towards 0 it is easy to deduce that

$$\int 1_F(x) \, Q(\phi, \nabla\phi, \nabla\psi_n) \, dx \underset{n}{\to} 0 .$$

We next consider the more general situation of a nucleus with N neutrons, Z protons (so $A = N + Z$). We may number the wave functions φ_i in such a way that $\varphi_1, \ldots, \varphi_N$ correspond to neutrons while $\varphi_{N+1}, \ldots, \varphi_A$ correspond to protons. We also denote by ρ_n, τ_n, $\rho_n(x, y)$ (resp. ρ_p, τ_p, $\rho_p(x, y)$) the various densities of neutrons (resp. protons) i.e.

$$\rho_n(x) = \sum_{i=1}^{N} |\varphi_i(x)|^2 , \qquad \tau_n(x) = \sum_{i=1}^{N} |\nabla\varphi_i(x)|^2 ,$$

$$\rho_n(x, y) = \sum_{i=1}^{N} \varphi_i(x) \, \varphi_i^*(y)$$

$$\rho_p(x) = \sum_{i=N+1}^{A} |\varphi_i(x)|^2 , \qquad \tau_p(x) = \sum_{i=N+1}^{A} |\nabla\varphi_i(x)|^2$$

$$\rho_p(x, y) = \sum_{i=N+1}^{A} \varphi_i(x) \, \varphi_i^*(y) .$$

In this general case, the functional to be minimized is

$$E(\varphi_1, \dots, \varphi_n) = \int_{\mathbb{R}^3} \frac{\hbar^2}{2m}\tau - \frac{t_0}{2}\left[\left(1 + \frac{x_0}{2}\right)\rho^2 - \left(x_0 + \frac{1}{2}\right)(\rho_n^2 + \rho_p^2)\right] +$$

$$+ \frac{\alpha}{4}\rho\tau - \frac{\beta}{4}(\rho_n \tau_n + \rho_p \tau_p) + \frac{\gamma}{16}|\nabla\rho|^2 - \frac{\delta}{16}(|\nabla\rho_n|^2 + |\nabla\rho_p|^2)$$

$$+ \frac{t_1}{3}\rho\rho_n\rho_p \, dx + \frac{e^2}{2}\int_{\mathbb{R}^3 \times}\int_{\mathbb{R}^3} \rho_p(x)\frac{1}{|x - y|}\rho_p(y)\, dx\, dy -$$

$$- \frac{e^2}{2} \times \int_{\mathbb{R}^3 \times}\int_{\mathbb{R}^3} \frac{1}{|x - y|}|\rho_p(x, y)|^2\, dx\, dy \tag{28}$$

where $e \in \mathbb{R}$, $t_0 > 0$, $x_0 \in (0, 1)$, $\alpha, \beta, \gamma, \delta, t_1 > 0$.

Observe that the last two terms obviously correspond to a Coulombic interaction between protons. Let us also mention that very often the last term (Coulomb exchange term) is neglected : this makes no difference on the type of mathematical results we prove. Still about the form of the functional it is worth remarking that the parameters α, β, γ, δ are not completely independent since in fact some of these terms are exchange terms.

The first situation we studied in this section corresponds to the situation when the Coulomb term is neglected ($e = 0$), $N = Z$ and $\rho_n = \rho_p = \frac{1}{2}\rho$, $\tau_n = \tau_p = \frac{1}{2}\tau$. Finally, we would like to remark that $E(\varphi_1, \dots, \varphi_A)$ is not invariant anymore under all unitary transforms of $(\varphi_1, \dots, \varphi_A)$ but only under the transforms of the form

$$U = \begin{pmatrix} U_n & 0 \\ 0 & U_p \end{pmatrix} \tag{29}$$

where U_n (resp. U_p) is a $N \times N$ (resp. $Z \times Z$) unitary matrix.

And we consider now the HF minimization problem

$$I = \mathrm{Inf}\left\{ E(\varphi_1, \dots, \varphi_A) \mid \varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho\tau\, dx < \infty, \right.$$

$$\left. \int_{\mathbb{R}^3} \varphi_i \varphi_j^*\, dx = \delta_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant N \quad \text{and for} \quad N + 1 \leqslant i, j \leqslant A \right\} \tag{30}$$

together with its extension

$$I_M = \operatorname{Inf}\left\{ E(\varphi_1, \dots, \varphi_A) \mid \varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho\tau \, dx < \infty , \right.$$

$$\left. \int_{\mathbb{R}^3} \varphi_i \, \varphi_j^* \, dx = m_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant N \quad \text{and for} \quad N + 1 \leqslant i, j \leqslant A \right\} \tag{31}$$

where $M = (m_{ij}) = \begin{pmatrix} M_n & 0 \\ 0 & M_p \end{pmatrix}$ is a block diagonal hermitian nonnegative matrix. Using unitary transforms of the form (29), it is clear that we may still diagonalize M into $\operatorname{diag}(m_1, \dots, m_A)$ where $m_i \geqslant 0$ for all $i \in \{ 1, \dots, A \}$. Therefore $I_M = I(m_1, \dots, m_A)$ where

$$I(m_1, \dots, m_A) = \operatorname{Inf}\left\{ E(\varphi_1, \dots, \varphi_A) \mid \varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho\tau \, dx < \infty , \right.$$

$$\left. \int_{\mathbb{R}^3} \varphi_i \, \varphi_j^* \, dx = m_i \, \delta_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant N \quad \text{and for} \quad N + 1 \leqslant i, j \leqslant A \right\}.$$

Observe also that the orthogonality conditions in (30) still enable us to write down Euler-Lagrange equations (the HF equations) where, up to a unitary transform of the form (29), the matrix of Lagrange multipliers (e_i in (17)) is diagonal and the Lagrange multipliers are eigenvalues of self-adjoint operators.

Before going further in the mathematical analysis of (30), we would like to mention the way the parameters t_0, t_1, x_0, α, β, γ, δ are chosen in realistic computations. The parameters are adjusted by a simple fit to the binding energies and equilibrium densities of some fixed nucleii (essentially oxygen-16 and lead-258). Once this fitting is performed (see the tables in D. Vautherin and D. M. Brink [46]), one can compute all other nucleii by solving numerically (30).

It is clear that conditions on the parameters are needed in order to insure that $I > -\infty$ (and that minimizing sequences are bounded). The boundedness of I and the solution of (30) are analyzed in the

THEOREM IV.4 : i) *Assume that* $\alpha > (\beta + \delta)/2$, $\alpha + \delta \wedge \gamma > \delta + \beta$. *Then for all* N, Z *the infimum* $I \in (-\infty, 0]$ *and for all* $R > 0$ *there exists* $C_R > 0$ *such that for all* $(\varphi_1, \dots, \varphi_A)$ *in the minimizing class satisfying* $E(\varphi_1, \dots, \varphi_A) \leqslant R$ *then* $\int_{\mathbb{R}^3} \rho + \tau + \rho\tau \, dx \leqslant C_R$.

ii) *Assume that* $\alpha < (\beta + \delta)/2$ *then, for all* N, $Z \geqslant 1$, $I = -\infty$.

iii) *Assume that the conditions given in* i) *hold. Then any minimizing sequence of* (30) *is relatively compact up to a translation if and only if the following condition holds*

$$I < I(m_1, \ldots, m_A) + I(1 - m_1, \ldots, 1 - m_A) \quad \textit{for all} \quad m_i \in [0, 1] \quad (1 \leqslant i \leqslant A) \tag{32}$$

such that $\sum_{i=1}^{A} m_i \in (0, A)$.

In particular, if (32) *holds, there exists a minimum of* (30).

Remarks : i) The analogues of the remarks given after Theorem IV.1 still hold here.

ii) There are other conditions than $\alpha < (\beta + \delta)/2$ which imply that $I = -\infty$. We mention only this one to emphasize the following phenomenon : take $N = Z$, $e = 0$ then in this case it is often assumed in the Physics litterature that it is enough to consider $(\varphi_1, \ldots, \varphi_A)$ such that $\rho_n = \rho_p = \frac{1}{2}\rho$, $\tau_n = \tau_p = \frac{1}{2}\tau$ without changing the value of I. And this is completely false in general (it would be certainly of interest to understand completely this kind of symmetry breaking). Indeed, choose $\alpha, \beta, \gamma, \delta > 0$ so that

$$\alpha < (\beta + \delta)/2, \quad (\alpha + \gamma) > (\beta + \delta)/2$$

then ii) implies that $I = -\infty$ while

$$\begin{aligned}\operatorname{Inf}\Big\{ & E(\varphi_1, \ldots, \varphi_A) \mid \varphi_i \in H^1, \int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij}, \int_{\mathbb{R}^3} \rho\tau \, dx < \infty, \\ & \rho_n = \rho_p = \frac{1}{2}\rho, \tau_n = \tau_p = \frac{1}{2}\tau \Big\} \geqslant \\ & \geqslant \operatorname{Inf}\Big\{ E'(\varphi_1, \ldots, \varphi_A) \mid \varphi_i \in H^1, \int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij}, \int_{\mathbb{R}^3} \rho\tau \, dx < \infty \Big\}\end{aligned}$$

where

$$E'(\varphi_1, \ldots, \varphi_A) = \int_{\mathbb{R}^3} \frac{\hbar^2}{2m}\tau - \frac{3\,t_0}{8}\rho^2 + \frac{1}{4}\left(\alpha - \frac{\beta}{2}\right)\rho\tau + \frac{1}{16}\left(\gamma - \frac{\delta}{2}\right)|\nabla\rho|^2 + \frac{t_1}{12}\rho^3 \, dx .$$

Hence, by part i) of Theorem IV.1, the restricted infimum is finite as soon as $(\alpha + \gamma) > (\beta + \delta)/2$.

Proof of Theorem IV.4 : We begin by proving part i). We first observe that we have denoting by $\gamma' = \gamma \wedge \delta$

$$\frac{\alpha}{4}\rho\tau - \frac{\beta}{4}(\rho_n\tau_n + \rho_p\tau_p) + \frac{\gamma}{16}|\nabla\rho|^2 - \frac{\delta}{16}(|\nabla\rho_n|^2 + |\nabla\rho_p|^2) \geqslant$$

$$\geqslant \frac{\alpha}{4}(\rho_n\tau_p + \rho_p\tau_n) + \frac{\alpha-\beta}{4}(\rho_n\tau_n + \rho_p\tau_p) + \frac{\gamma'}{8}(\nabla\rho_n, \nabla\rho_p) + - \frac{\delta-\gamma'}{16}(|\nabla\rho_n|^2 + |\nabla\rho_p|^2).$$

But $|\nabla\rho_n|^2 \leqslant 4\rho_n\tau_n$, $|\nabla\rho_p|^2 \leqslant 4\rho_p\tau_p$, and

$$|(\nabla\rho_n, \nabla\rho_p)| \leqslant 2(\rho_n\tau_n + \rho_p\tau_p), \qquad |(\nabla\rho_n, \nabla\rho_p)| \leqslant 2(\rho_p\tau_n + \rho_n\tau_p)$$

so the above quantity is bounded from below by

$$\left(\frac{\alpha+\gamma'-\beta-\delta}{4}\right)(\rho_n\tau_n + \rho_p\tau_p) + \frac{\alpha}{4}(\rho_n\tau_p + \rho_p\tau_n) - - \frac{\gamma'}{8}|(\nabla\rho_n, \nabla\rho_p)| \geqslant \nu\rho\tau$$

where ν is a positive constant. And this yields

$$E(\varphi_1, \dots, \varphi_A) \geqslant \int_{\mathbb{R}^3} \frac{\hbar^2}{2m}\tau + \nu\rho\tau - C\rho^2\,dx + - \frac{e^2}{2}\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3} \frac{1}{|x-y|}|\rho_p(x,y)|^2\,dx\,dy$$

for some $C \geqslant 0$ (depending only on t_0, x_0). Next, we remark that $|\rho_p(x,y)|^2 \leqslant \rho_p(x)\,\rho_p(y)$ and thus by standard convolution inequalities

$$\frac{e^2}{2}\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3}\frac{1}{|x-y|}|\rho_p(x,y)|^2\,dx\,dy \leqslant C\|\rho_p\|^2_{L^{6/5}(\mathbb{R}^3)} \leqslant$$

$$\leqslant C\|\rho\|^{3/2}_{L^1(\mathbb{R}^3)}\|\rho\|^{1/2}_{L^3(\mathbb{R}^3)} \leqslant C\left(\int_{\mathbb{R}^3}\sum_i|\varphi_i|^6\,dx\right)^{1/6}$$

and by Sobolev inequalities

$$\leqslant C\left(\sum_i\int_{\mathbb{R}^3}|\nabla\varphi_i|^2\,dx\right)^{1/2} = C\left(\int_{\mathbb{R}^3}\tau\,dx\right)^{1/2}$$

where C denotes various constants depending only on e and A. Therefore, one gets

$$E(\varphi_1, \ldots, \varphi_A) \geqslant \frac{\hbar^2}{2m}\int_{\mathbb{R}^3} \tau \, dx + \nu \int_{\mathbb{R}^3} \rho\tau \, dx - C\int_{\mathbb{R}^3} \rho^2 \, dx + \\ - C\left(\int_{\mathbb{R}^3} \tau \, dx\right)^{1/2}.$$

It just remains to bound conveniently $\int_{\mathbb{R}^3} \rho^2 \, dx$. In the computations that follow C denotes various constants depending only on A :

$$\begin{aligned}\int_{\mathbb{R}^3} \rho^2 \, dx &\leqslant C \sum_i \int_{\mathbb{R}^3} |\varphi_i|^4 \, dx \\ &\leqslant C\left(\sum_i \int_{\mathbb{R}^3} |\varphi_i|^2 \, dx\right)^{4/5} \left(\sum_i \int_{\mathbb{R}^3} |\varphi_i|^{12} \, dx\right)^{1/5}\end{aligned}$$

by Hölder inequalities, and since $\int_{\mathbb{R}^3} |\varphi_i|^2 \, dx = 1$ for all i

$$\begin{aligned}&\leqslant C\left(\int_{\mathbb{R}^3} \rho^6 \, dx\right)^{1/5} \\ &\leqslant C\left(\int_{\mathbb{R}^3} |\nabla\rho|^2 \, dx\right)^{3/5} \quad \text{by Sobolev inequalities} \\ &\leqslant C\left(\int_{\mathbb{R}^3} \rho\tau \, dx\right)^{3/5}.\end{aligned}$$

This allows us to conclude the proof of part i).

The proof of part iii) is the same as the proof of Theorem IV.1 and thus we will skip it. To prove part ii) we have to build appropriate test functions. By simple considerations it is enough to treat the case $N = Z = 1$ so denoting $\varphi = \varphi_1, \psi = \varphi_2$ we have $\rho_n = \varphi^2, \rho_p = \psi^2$ since we will take real-valued φ, ψ. We construct spherically symmetric functions φ^m, ψ^m as follows. Let $t_0 > 1$ be such that $\left[\frac{\beta + \delta}{2} - \alpha\right] t_0^2 > \frac{\hbar^2}{m}$, let $\delta_0 > 0$, $r_0 > 0$: δ_0, r_0 will have to be determined later on and we assume at least $\delta_0 < 1/4$, $r_0 < 1$. We are going to build first φ^m, ψ^m in the ball $B(0, r_0)$: ψ^m will take values in the interval

$[t_0 - \delta_0, t_0]$ and $\varphi^m = (2\,t_0^2 - (\psi^m)^2)^{1/2}$. We next compute on the ball $B(0, r_0)$

$$\frac{\hbar^2}{2\,m}\tau^m + \frac{\alpha}{4}\rho^m\tau^m - \frac{\beta}{4}(\rho_n^m\tau_n^m + \rho_p^m\tau_p^m) + \frac{\gamma}{16}|\nabla\rho^m|^2 - \frac{\delta}{16}(|\nabla\rho_n^m|^2 + $$

$$+ |\nabla\rho_p^m|^2) \leqslant |\nabla\psi^m|^2\left\{\frac{\hbar^2}{m} + \frac{\alpha}{4}(1 + (F')^2)\rho^m - \frac{\beta+\delta}{4}((\varphi^m)^2(F')^2 + (\varphi^m)^2)\right\}$$

where $F(t) = (2\,t_0^2 - t^2)^{1/2}$. Now for δ_0 small enough $|F'|$ takes values as close to 1 as we wish while $(\varphi^m)^2$, $(\psi^m)^2$ take values arbitrarily close to t_0^2. Therefore fixing $\delta_0 > 0$ small enough the quantity between brackets is bounded by $-\nu$ with $\nu > 0$, Since we will extend φ^m, ψ^m outside $B(0, r_0)$ in such a way that φ^m, ψ^m and their first derivatives are bounded by fixed constants (depending only on t_0) and have compact support say in $B(0, 1)$ we deduce

$$E(\varphi^m, \psi^m) \leqslant -\nu\int_{B(0,r_0)}|\nabla\psi^m|^2\,dx + C\,.$$

Now, we choose t_0 by imposing $\{\,t_0^2 + F(t_0 - \delta_0)^2\,\}\dfrac{4\,\pi r_0^3}{3} \leqslant 1/8$, and we define ψ^m as follows on $B(0, r_0)$

$$\psi^m(x) = t_0 - \delta_0 \quad \text{if} \quad |x| \leqslant \frac{r_0}{2} - \frac{1}{2\,m}, \quad = r_0 \quad \text{if} \quad |x| \geqslant \frac{r_0}{2} + \frac{1}{2\,m}$$

$$= t_0 - \delta_0/2 + \delta_0\,m\left(|x| - \frac{r_0}{2}\right) \quad \text{if} \quad \frac{r_0}{2} - \frac{1}{2\,m} \leqslant |x| \leqslant \frac{r_0}{2} + \frac{1}{2\,m}.$$

It is of course easy to extend φ^m, ψ^m outside $B(0, r_0)$ as we claimed above and we can even do so imposing

$$\int_{\mathbb{R}^3}(\varphi^m)^2\,dx = 1, \int_{\mathbb{R}^3}(\psi^m)^2\,dx = 1, \int_{\mathbb{R}^3}\varphi^m\,\psi^m\,dx = 0$$

(this is where we use the restriction on r_0). Computing

$$\int_{B(0,r_0)}|\nabla\psi^m|^2\,dx = \delta_0^2\,m^2\,\frac{4\,\pi}{3}\left[\left(\frac{r_0}{2} + \frac{1}{2\,m}\right)^3 - \left(\frac{r_0}{2} - \frac{1}{2\,m}\right)^3\right] \underset{m}{\to} +\infty$$

we prove that $E(\varphi^m, \psi^m) \underset{m}{\to} -\infty$. ∎

Remarks : i) Let us observe that even if we restrict in ii) the infimum to spherically symmetric functions, the infimum is $-\infty$.

ii) The idea of the above tedious constructions is to choose at least locally near 0, $\rho = \varphi^2 + \psi^2$ constant, $|\nabla\varphi|^2 \sim |\nabla\psi|^2$, $\varphi^2 \sim \psi^2$, thus cancelling the $\gamma\,|\nabla\rho|^2$ term while making the other terms

$$\alpha\rho\tau - \beta(\rho_n\tau_n + \rho_p\tau_p) - \frac{\delta}{4}(|\nabla\rho_n|^2 + |\nabla\rho_p|^2)$$

approximately equal to $\left(\alpha - \frac{\beta}{2} - \frac{\delta}{2}\right)\rho\tau$ ■

We would like to conclude this section by emphasizing Remark ii) following it is a priori not correct in general to restrict the infimum to configurations such that $\tau_n = \tau_p = \frac{1}{2}\tau$, $\rho_n = \rho_p = \frac{1}{2}\rho$ In fact, we gave an example of a dramatic symmetry breaking in the isospin variable (between n and p i e between neutrons and protons) Of course, a precise study of this phenomenon (maybe on simpler model problems) certainly remains to be made, investigating in particular the possible bifurcations corresponding to it From the Physics viewpoint, this symmetry breaking does not seem to have been observed for nuclei such that $N = Z$ in particular because realistic computations take into account the Coulomb force between protons (and thus the symmetry is not really satisfied) However, it would be interesting to look for related effects such as metastable states or local minima

V. OTHER INTERACTIONS

We have considered in the preceding sections the case of the Skyrme's interaction which basically corresponds to the choice (5) (in fact the difference between neutrons and protons wave functions φ_i in the preceding section comes from the fact that wave functions should depend on the so-called isospin variable which takes fixed different values for neutrons or protons and that the Hamiltonian acts also on this isospin variable) It is easy to understand that (5) is a very simplistic model of nuclear interactions which, even if they have a short range, do not have " zero-range " However this model is often used because it already gives reasonably good numerical results and the HF equations being completely local are somewhat easier to compute Nevertheless the theories allowing to derive the effective interaction V from first principle reveal that one has to consider more sophisticated parametrization (i e different V) Furthermore several extensions of the HF theory (as for example time dependent Hartree-Fock problems, Hartree-Fock-Bogolyubov theory) make necessary the use of more realistic interactions V On all these basic issues, we refer to J Negele [43]

In this section we are mainly interested in the case when V is given by (3) even if it is quite clear that most of the arguments we present below are still valid for much more general V (including (4) as another example). We will not bother to indicate precisely what are the mathematical assumptions we need : it is an easy exercise to figure out in which $L^p + L^q$ class (for instance) one has to take V and we leave it to the reader.

Again to explain the difficulties encountered, we begin with the scalar case which more or less corresponds to the case of the alpha particle. For V given by (3), we introduce the functional

$$E(\varphi) = \frac{\hbar^2}{2\,m}\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx + t_0\int_{\mathbb{R}^3} |\varphi|^{4+2/3} + \\ + \frac{1}{4}\int_{\mathbb{R}^3}\times\int_{\mathbb{R}^3} |\varphi|^2(x)\,V(x-y)\,|\varphi|^2(y)\,dx\,dy \quad (33)$$

where $t_0 > 0$. Observe that we also changed the type of nonlinear terms. And we want to study the following minimization problem

$$I = \mathrm{Inf}\left\{ E(\varphi)/\varphi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\varphi|^2\,dx = 1 \right\} \quad (34)$$

that we embed in the following family of problems

$$I_\lambda = \mathrm{Inf}\left\{ E(\varphi)/\varphi \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |\varphi|^2\,dx = \lambda \right\} \quad (35)$$

where λ is a positive parameter. In fact solving (35) for some $\lambda > 0$ amounts to solve (34) for different values of $\frac{\hbar^2}{2\,m}$, t_0, α, β as it is easily seen by a scaling argument. We begin by a simple observation

PROPOSITION V.1 : i) *For all* $R < \infty$, *there exists* $C_R < \infty$ *such that* $\|\varphi\|_{H^1(\mathbb{R}^3)} \leqslant C_R$ *if* $\varphi \in H^1(\mathbb{R}^3)$, $E(\varphi) \leqslant R$, $\int_{\mathbb{R}^3} |\varphi|^2\,dx \leqslant R$.

ii) *One has always* $I_\lambda \leqslant 0$. *If* $\alpha, \beta > 0$, $I_\lambda = 0$ *for all* $\lambda > 0$ *and there is no minimum of* (35).

iii) *There exists* $\lambda_0 \in (0, +\infty]$ *such that* $I_\lambda = 0$ *for* $\lambda \leqslant \lambda_0$, $I_\lambda < 0$ *for* $\lambda > \lambda_0$.

iv) *If* $\frac{\alpha}{\mu^{N/2}} + \frac{\beta}{\nu^{N/2}} < 0$, *then* $\lambda_0 < \infty$.

Proof: Part i) is easy and we skip it. If $\alpha, \beta > 0$, $E(\varphi) > 0$ for all $\varphi \neq 0$ and thus admitting $I_\lambda \leqslant 0$ the remainder of ii) is clear. To prove that $I_\lambda \leqslant 0$, we consider $\varphi \in \mathscr{D}(\mathbb{R}^3)$ such that $\int_{\mathbb{R}^3} |\varphi|^2\,dx = \lambda$ and we denote by $\varphi_\sigma(x) = \varphi\left(\frac{x}{\sigma}\right)\sigma^{-3/2}$. Computing $E(\varphi_\sigma)$ we find

$$E(\varphi_\sigma) = \frac{1}{\sigma^2}\left\{\frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx\right\} + \frac{1}{\sigma^4}\left\{t_0\int_{\mathbb{R}^3} |\varphi|^{4+2/3}\,dx\right\} + \\ + \frac{1}{4}\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3} |\varphi|^2\,(x)\,V(\sigma(x-y))\,|\varphi|^2\,(y)\,dx\,dy$$

hence $E(\varphi_\sigma) \to 0$ as $\sigma \to \infty$.

To prove iii), one first remarks that I_λ is nonincreasing since by the concentration-compactness argument one has always

$$I_\lambda \leqslant I_\gamma + I_{\lambda-\gamma} \quad \text{for all} \quad \gamma \in (0, \lambda) \tag{36}$$

and $I_{\lambda-\gamma} \leqslant 0$. Therefore one just has to prove that $I_\lambda = 0$ for λ small enough. Indeed if $\varphi \in H^1(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} |\varphi|^2\,dx = \lambda$

$$\left|\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3} |\varphi|^2(x)\,V(x-y)\,|\varphi|^2(y)\,dx\,dy\right| \leqslant \\ \leqslant \|\varphi\|^2_{L^6(\mathbb{R}^3)}\,\|\varphi\|^2_{L(\mathbb{R}^3)}\,\|V\|_{L^{3/2}(\mathbb{R}^3)} \leqslant C\lambda\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx$$

so for λ small enough $E(\varphi) \geqslant 0$ and iii) is proved.

The proof of iv) relies on the following choice of φ : take $\varphi \in \mathscr{D}(\mathbb{R}^3)$ and set $\varphi_\sigma(x) = \sigma^{-3/4}\,\varphi\left(\frac{x}{\sigma}\right)$. Then computing $E(\tilde{\varphi}_\sigma)$ we find

$$E(\tilde{\varphi}_\sigma) = \sigma^{-1/2}\left\{\frac{\hbar^2}{2m}\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx\right\} + \sigma^{-1/2}\left\{t_0\int_{\mathbb{R}^3} |\varphi|^{4+2/3}\,dx\right\} + \\ + \frac{1}{4}\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3} |\varphi|^2\,(x)\,|\varphi|^2\,(y)\,\{\,\sigma^3\,V(\sigma(x-y))\,\}\,dx\,dy\,.$$

Remark that $\sigma^3 V(\sigma x) \to \left(\frac{\alpha}{\mu^{N/2}} + \frac{\beta}{\nu^{N/2}}\right) \pi^{N/2} \delta_0(x)$ in $\mathscr{D}'(\mathbb{R}^3)$ as $\sigma \to \infty$ and we conclude easily letting σ go to $+\infty$ ■

We next give a result concerning the solution of (35)

THEOREM V 2 i) *Every minimizing sequence of* (35) *is relatively compact in* $H^1(\mathbb{R}^3)$ *up to a translation if and only if the following condition holds*

$$I_\lambda < I_\gamma + I_{\lambda-\gamma}, \quad \text{for all} \quad \gamma \in (0, \lambda) \tag{37}$$

In particular if (37) *holds there exists a minimum of* (35)

ii) *If* $\alpha, \beta < 0$ *and if the following condition holds*

$$I_\lambda < I_\gamma, \quad \text{for all} \quad \gamma \in (0, \lambda) \tag{38}$$

then there exists a minimum of (35) *which is spherically symmetric, nonnegative, smooth and decreasing with respect to* $|x|$

Remarks i) Very little is known on the values of λ (or equivalently α, β, $t_0, \frac{\hbar^2}{2m}$) for which (37) or (38) holds We only got very partial results on this important question

ii) If for some $\lambda_0 > 0$, (38) holds and (37) does not hold then there exists a minimum of (35) while some minimizing sequences are not relatively compact even up to a translation If this were to happen this would be an extremely interesting situation

Proof of Theorem V 2 Part i) is proved by a direct application of the concentration-compactness arguments [33] To prove part ii) we first observe that by a somewhat standard symmetrization argument (as in E H Lieb [28], H Berestycki and P L Lions [5]) one sees that I_λ agrees with the infimum of $E(\varphi)$ for $\varphi \in H^1(\mathbb{R}^3)$, φ spherically symmetric, nonincreasing with respect to $|x|$, nonnegative and $\int_{\mathbb{R}^3} |\varphi|^2 \, dx = \lambda$ Therefore, it is enough to prove that if (38) holds then there exists a minimum of $I_\lambda^s = \operatorname{Inf}\left\{ E(\varphi)/\varphi \in H^1(\mathbb{R}^3), \varphi \text{ is spherically symmetric}, \int_{\mathbb{R}^3} |\varphi|^2 \, dx = \lambda \right\}$, the other properties of the minimum following easily Now to solve I_λ^s we may either apply the concentration-compactness arguments in presence of symmetries (see [34]) and conclude observing that since I_λ vanishes for λ small then $\lim_n n I_{\lambda/n} = 0$ for all $\lambda > 0$ and thus (38) is equivalent to $I_\lambda^s = I_\lambda < I_\gamma^s + \lim_n n I_{(\lambda-\gamma)/n}$ or we may use a more standard line of arguments showing first (as in [28], [46], [5]) that there exists a minimum φ_0 of $\operatorname{Inf}\left\{ E(\varphi)/\varphi \in H^1(\mathbb{R}^3),\ \varphi \text{ is spherically symmetric}, \int_{\mathbb{R}^3} |\varphi|^2\, dx \leqslant \lambda \right\}$ and concluding that $\int_{\mathbb{R}^3} |\varphi_0|^2\, dx = \lambda$ since (38) holds ∎

Before going into the general case, we study problems like (35) with $\hbar = 0$ in which case (35) reduces to

$$I_\lambda = \operatorname{Inf}\left\{ t_0 \int_{\mathbb{R}^3} |\varphi|^{4+2/3}\, dx + \frac{1}{4}\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3} |\varphi|^2(x)\, V(x-y)\, |\varphi|^2(y)\, dx\, dy \right.$$
$$\left. \varphi \in L^2(\mathbb{R}^3) \cap L^{14/3}(\mathbb{R}^3),\ \int |\varphi|^2\, dx = \lambda \right\} \quad (39)$$

$\left(\text{in fact the value } \frac{14}{3} \text{ plays no role in the analysis below, for example everything below remains true if we replace } \frac{14}{3} \text{ by any } \sigma > 4\right)$ We still denote by $E(\varphi)$ the functional that we wish to minimize We can prove the

THEOREM V 3 i) *If for any $\rho \in L^1(\mathbb{R}^3)$, $\rho \geqslant 0$ we have*

$$\int_{\mathbb{R}^3\times}\int_{\mathbb{R}^3} \rho(x)\, V(x-y)\, \rho(y)\, dx\, dy \geqslant 0 \quad (40)$$

then $I = 0$ for all $\lambda > 0$ and there is no minimum of (39) On the other hand, if (40) does not hold for some $\rho \in L^1(\mathbb{R}^3)$, $\rho \geqslant 0$ then $I_\lambda < 0$ for all $\lambda > 0$ This is the case if, for example, $\alpha + \beta < 0$ or $\frac{\alpha}{\mu^{N/2}} + \frac{\beta}{\nu^{N/2}} < 0$ In all that follows we assume that $I_\lambda < 0$ for all $\lambda > 0$

ii) *Every minimizing sequence of (39) is bounded in $L^2(\mathbb{R}^3) \cap L^{14/3}(\mathbb{R}^3)$*

iii) *Every minimizing sequence of (39) is relatively compact in $L^2(\mathbb{R}^3) \cap L^{14/3}(\mathbb{R}^3)$ up to a translation if and only if (37) holds In particular if (37) holds there is a minimum of (39)*

iv) *The condition (37) holds if λ is small enough*

v) *If α and β are negative, (37) holds for all $\lambda > 0$ and there is a minimum of (39) which is spherically symmetric, nonnegative, nonincreasing with respect to $|x|$ and with compact support*

Remarks 1) If we assume that (37) holds at $\lambda > 0$ then we can prove that either (37) holds in a neighborhood of λ or there exists a minimum of (39) that we denote by φ_0 — such that $\varphi_0 \in L^2(\mathbb{R}^3) \cap L^{14/3}(\mathbb{R}^3)$ and

$$E'(\varphi_0) = 0 \quad \text{i.e.} \quad \frac{14}{3} t_0\, \varphi_0^{11/3} = \varphi_0(\varphi_0^2 * V) \quad \text{a.e. in } \mathbb{R}^3 \tag{41}$$

(we may always assume that φ_0 is real-valued, nonnegative).

Indeed, if for any minimum of (39), (41) does not hold then, assuming that we have built a sequence $\gamma_n \underset{n}{\to} \lambda$ such that (37) holds for I_{γ_n} and denoting by φ_n the associated minima, on one hand φ_n converges (up to subsequences) in $L^{14/3}(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ to some minimum φ_0 of I_λ and on the other hand there exists θ_n satisfying

$$E'(\varphi_n) + \theta_n\, \varphi_n = 0 \quad \text{a.e. in } \mathbb{R}^3, \quad 0 < \nu \leqslant \theta_n \leqslant C \tag{42}$$

for some positive constants ν, C.

Now we argue by contradiction : if (37) does not hold for I_{λ_n} where $\lambda_n \underset{n}{\to} \lambda$, then there exists $\gamma_n \geqslant \lambda_n/2$ such that

$$I_{\lambda_n} = I_{\gamma_n} + I_{\lambda_n - \gamma_n}, \quad 0 < \gamma_n < \lambda_n$$

and since (37) holds for I_γ we have that $\gamma_n \underset{n}{\to} \lambda$. Next, if (37) does not hold for I_{γ_n}, there would exist $\delta_n \in [\gamma_n/2, \gamma_n)$ such that $I_{\gamma_n} = I_{\delta_n} + I_{\gamma_n - \delta_n}$. In particular we have

$$I_{\lambda_n} = I_{\gamma_n} + I_{\lambda_n - \gamma_n} = I_{\delta_n} + I_{\gamma_n - \delta_n} + I_{\lambda_n - \gamma_n}.$$

But we always have

$$I_{\gamma_n - \delta_n} + I_{\lambda_n - \gamma_n} \geqslant I_{\lambda_n - \delta_n}, \quad I_{\delta_n} + I_{\lambda_n - \delta_n} \geqslant I_{\lambda_n}$$

so the above equality yields

$$I_{\lambda_n} = I_{\delta_n} + I_{\lambda_n - \delta_n}, \quad I_{\lambda_n - \delta_n} = I_{\gamma_n - \delta_n} + I_{\lambda_n - \gamma_n}.$$

Since (37) holds for I_γ, the first equality implies that $\delta_n \underset{n}{\to} \lambda$. But then the second equality gives a contradiction since (37) holds for λ small enough. Therefore (37) holds for I_{γ_n}.

To conclude we argue as in [34] : observe that by (42)

$$\begin{aligned} I_{\gamma_n} + I_{\lambda_n - \gamma_n} = I_{\lambda_n} &\leqslant E\left[\left(\frac{\lambda_n}{\gamma_n}\right)^{1/2} \varphi_n\right] \simeq E(\varphi_n) + \left\{\left(\frac{\lambda_n}{\gamma_n}\right)^{1/2} - 1\right\} E'(\varphi_n).\varphi_n \\ &\leqslant I_{\gamma_n} - K(\lambda_n - \gamma_n) \end{aligned}$$

for some $K > 0$ (the almost equal sign can be easily justified and the above inequality holds rigorously). On the other hand, we prove below that $I_\lambda \lambda^{-2}$ converges to a negative constant as λ goes to 0. Hence we get

$$K(\lambda_n - \gamma_n) \leqslant C(\lambda_n - \gamma_n)^2$$

and the contradiction proves our claim.

2) We would like to remark also that, if we do not assume that α and β are negative, the question of the spherical symmetry of the minimum of (39) (when it exists, as for example when λ is small) is open.

3) Let us finally point out that somewhat related problems are considered in J. F. G. Auchmuty and R. Beals [1], [2], P. L. Lions [36], [33].

Proof of Theorem V.3 : The proofs of i) and ii) are standard : the sign question being a consequence of the difference of homogeneity of the two terms in E, and the negativity of I_λ when $\alpha\mu^{-N/2} + \beta\nu^{-N/2} < 0$ being proved as in Proposition V.1. Part iii) is proved by a simple application of the concentration-compactness method.

We now prove part iv). We first show that

$$I_\lambda \lambda^{-2} \underset{\lambda \to 0}{\to} \bar{I} = \operatorname{Inf}\left\{ \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |\varphi|^2(x) V(x-y) |\varphi|^2(y)\, dx\, dy \,/\, \varphi \in L^2(\mathbb{R}^3),\ \int_{\mathbb{R}^3} |\varphi|^2 dx = 1 \right\}. \quad (43)$$

Observe by the way that the infimum in $\bar{I}$ is achieved by a simple application of the concentration-compactness principle. To prove (43) it is enough to remark that on one hand $I_\lambda \geqslant \lambda^2 \bar{I}$ while on the other hand choosing $\varphi_n \in \mathscr{D}(\mathbb{R}^3)$ such that

$$\bar{I} \leqslant E_2(\varphi_n) = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |\varphi_n|^2(x) V(x-y) |\varphi_n|^2(y)\, dx\, dy \leqslant \bar{I} + \frac{1}{n}$$

and $\int_{\mathbb{R}^3} |\varphi_n|^2 dx = 1$, we obtain

$$I_\lambda \leqslant E[\sqrt{\lambda}\varphi_n] \leqslant C_n \lambda^{2+1/3} + \lambda^2\left(\bar{I} + \frac{1}{n}\right).$$

Next, let us argue by contradiction to prove part iv) : assume there exist $\lambda_n \underset{n}{\to} 0$ and $\gamma_n \in (0, \lambda_n)$ such that

$$I_{\lambda_n} = I_{\gamma_n} + I_{\lambda_n - \gamma_n}. \quad (44)$$

This yields

$$\frac{I_{\lambda_n}}{\lambda_n^2} = \frac{I_{\gamma_n}}{\gamma_n^2}\left(\frac{\gamma_n}{\lambda_n}\right)^2 + \frac{I_{\lambda_n-\gamma_n}}{\lambda_n-\gamma_n}\left(\frac{\lambda_n-\gamma_n}{\lambda_n}\right)^2,$$

and this combined with (43) implies that up to subsequences $\frac{\gamma_n}{\lambda_n}$ converges either to 1 or to 0. Replacing if necessary γ_n by $\lambda_n - \gamma_n$ we may always assume that γ_n/λ_n converges to 1. Next, we fix n and we take a minimizing sequence φ_k for I_{γ_n}. We remark that

$$I_{\lambda_n} \leqslant \varliminf_k E\left[\left(\frac{\lambda_n}{\gamma_n}\right)^{1/2}\varphi_k\right] = \varliminf_k \left\{\left(\frac{\lambda_n}{\gamma_n}\right)^{2+1/3} E_1(\varphi_k) + \left(\frac{\lambda_n}{\gamma_n}\right)^2 E_2(\varphi_k)\right\}$$

where we denote by $E_1(\varphi) = t_0 \int_{\mathbb{R}^3} |\varphi|^{4+2/3}\,dx$. On the other hand $E_1(\varphi_k) + E_2(\varphi_k) \underset{k}{\to} I_{\gamma_n}$ so we obtain

$$I_{\gamma_n} \leqslant \left(\frac{\lambda_n}{\gamma_n}\right)^{2+1/3} I_{\gamma_n} + \varliminf_k \left\{E_2(\varphi_k)\left(\left(\frac{\lambda_n}{\gamma_n}\right)^2 - \left(\frac{\lambda_n}{\gamma_n}\right)^{2+1/3}\right)\right\}$$

$$\leqslant I_{\gamma_n} + \left(\left(\frac{\lambda_n}{\gamma_n}\right)^2 - 1\right) I_{\gamma_n} + \varliminf_k \left\{(I_{\gamma_n} - E_2(\varphi_k))\left(\frac{\lambda_n}{\gamma_n}\right)^2\left(\left(\frac{\lambda_n}{\gamma_n}\right)^{1/3} - 1\right)\right\}.$$

Recalling (44) we deduce finally

$$I_{\lambda_n-\gamma_n} \leqslant \left(\left(\frac{\lambda_n}{\gamma_n}\right)^2 - 1\right) I_{\gamma_n} + \left(\frac{\lambda_n}{\gamma_n}\right)^2\left\{\left(1 + \frac{\lambda_n-\gamma_n}{\gamma_n}\right)^{1/3} - 1\right\} \times \varliminf_k \,(I_{\gamma_n} - E_2(\varphi_k)).$$

Of course $\varliminf_k \{I_{\gamma_n} - E_2(\varphi_k)\}$ depends on γ_n and similar arguments to those used to prove (43) show that

$$\varliminf_k \{I_{\gamma_n} - E_2(\varphi_k)\}\,\gamma_n^{-2} \underset{n}{\to} 0.$$

Next since $\frac{I_{\lambda_n-\gamma_n}}{(\lambda_n-\gamma_n)\gamma_n} = \frac{I_{\lambda_n-\gamma_n}}{(\lambda_n-\gamma_n)^2}\,\frac{\lambda_n-\gamma_n}{\gamma_n} \underset{n}{\to} 0$ dividing the above inequality by $(\lambda_n - \gamma_n)\gamma_n$ we obtain passing to the limit : $0 \leqslant 2I$, contradicting the negativity of I. And the contradiction proves iv).

We now conclude the proof of Theorem V.3 by proving part v). The proof involves several steps : 1) we show the existence of a spherically symmetric, nonincreasing minimum of (37), 2) that such minima have compact support. It is easy to conclude that (37) holds by observing that if φ_1, φ_2 are the respective minima of I_γ, $I_{\lambda-\gamma}$ for some $\gamma \in (0, \lambda)$ and if say φ_1, φ_2 are supported in a ball of radius R then considering

$$\tilde{\varphi}(x) = \varphi_1(x) + \varphi_2(x + 2\,Re)$$

where e is any unit vector, we obtain

$$\int_{\mathbb{R}^3} |\tilde{\varphi}|^2\,dx = \int_{\mathbb{R}^3} |\varphi_1|^2\,dx + \int_{\mathbb{R}^3} |\varphi_2|^2\,dx = \lambda$$

$$E(\tilde{\varphi}) = E(\varphi_1) + E(\varphi_2) + \frac{1}{2}\int_{\mathbb{R}^3}\times\int_{\mathbb{R}^3} \varphi_1(x)\,V(x-y)\,\varphi_2(y + 2\,Re)\,dx\,dy$$

and (37) is proved. (Observe that $\varphi_1, \varphi_2 \geqslant 0$ and $V < 0$.)

To prove 1) we argue as in the proof of Theorem V.2 introducing the problem in $\rho = |\varphi|^2$

$$I_\lambda = \operatorname{Inf}\left\{ t_0 \int_{\mathbb{R}^3} |\rho|^{7/3}\,dx + \frac{1}{4}\int_{\mathbb{R}^3}\times\int_{\mathbb{R}^3} \rho(x)\,V(x-y)\,\rho(y)\,dx\,dy \Big/ \right.$$
$$\rho \text{ spherically symmetric}, \quad \rho \in L^1(\mathbb{R}^3) \cap L^{7/3}(\mathbb{R}^3),$$
$$\left. \rho \geqslant 0 \text{ a.e.}, \quad \int_{\mathbb{R}^3} \rho\,dx \leqslant \lambda \right\}.$$

Then this problem is solved exactly as in P. L. Lions [36] using the spherical symmetry and the smoothing properties of the kernel $V(x-y)$; and there exists a minimum ρ_0 which is nonincreasing (using again symmetrization arguments). If we prove that $\int_{\mathbb{R}^3} \rho_0\,dx = \lambda$ then Step 1) is completed considering $\varphi_0 = \sqrt{\rho_0}$. In order to do so we argue by contradiction and we assume that $\int_{\mathbb{R}^3} \rho_0\,dx < \lambda$. Then the necessary conditions for minimality may be written as

$$\begin{cases} \frac{7}{3} t_0\,\rho_0^{4/3} + \frac{1}{2}(\rho_0 * V) = 0 & \text{a.e. on the set } \{\rho_0 > 0\} \\ \frac{7}{3} t_0\,\rho_0^{4/3} + \frac{1}{2}(\rho_0 * V) \geqslant 0 & \text{a.e. on the set } \{\rho_0 = 0\}. \end{cases}$$

But ρ_0 is spherically symmetric, nonincreasing with respect to $|x|$ so the set $\{\rho_0 > 0\}$ is a ball (up to zero measure sets) possibly $\mathbb{R}^3$ itself. If this ball is not $\mathbb{R}^3$, on its complement the above conditions yield $\rho_0 * V \geqslant 0$ and this is absurd since $\rho_0 \geqslant 0$, $\rho_0 \equiv 0$ and $V < 0$ in $\mathbb{R}^3$. Therefore $\{\rho_0 > 0\} = \mathbb{R}^3$ and

$$\frac{14}{3} t_0 \rho_0^{4/3}(x) = \int_{\mathbb{R}^3} \rho_0(y) \{ |\alpha| e^{-\mu|x-y|^2} + |\beta| e^{-\nu|x-y|^2} \} dy$$
$$\geqslant \left\{ \int_{|y| \leqslant |x|} |\alpha| e^{-\mu|x-y|^2} + |\beta| e^{-\nu|x-y|^2} dy \right\} \rho_0(x)$$

since ρ_0 is radial nonincreasing. A simple computation shows that the above integral is bounded away from 0 as $|x| \to \infty$ and we obtain a contradiction since $\rho_0 \to 0$ as $|x| \to \infty$, $\rho_0(x) > 0$ on $\mathbb{R}^3$. Hence step 1) is proved.

The proof of step 2) uses similar arguments : indeed let φ_0 be the above minimum ($\varphi_0 = \sqrt{\rho_0}$), φ_0 satisfies for some Lagrange multiplier $\theta > 0$

$$\frac{14}{3} t_0 \varphi_0^{11/3} + \varphi_0(\varphi_0^2 * V) + \theta\varphi_0 = 0 \quad \text{in } \mathbb{R}^3 .$$

If φ_0 does not have compact support, since φ_0 is radial nonincreasing we deduce that

$$\varphi_0(x) > 0 \text{ on } \mathbb{R}^3 , \quad \varphi_0 \to 0 \quad \text{as} \quad |x| \to \infty .$$

Dividing the above equality by φ_0 and letting $|x|$ go to ∞ we obtain $\theta = 0$. Then, $\rho_0 = \varphi_0^2$ satisfies the same properties as in the proof of step 1) and we reach a contradiction thus proving our claim.

We now conclude this section by considering the general case of functionals like (33) for less simplistic nucleii : we introduce the following functional (which, except for the distinction between neutrons and protons, basically corresponds to the potential V given by (3))

$$E(\varphi_1, \dots, \varphi_A) = \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} \tau \, dx + \frac{1}{4} \sum_{i=1,2} \left\{ W_i \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho(x) V_i(x-y) \times \right.$$
$$\times \rho(y) \, dx \, dy - H_i \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} \rho_n(x) V_i(x-y) \rho_n(y) \, dx \, dy -$$
$$\left. - H_i \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} \rho_p(x) V_i(x-y) \rho_p(y) \, dx \, dy \right\} +$$

$$- \frac{1}{4} \sum_{i=1,2} \left\{ M_i \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V_i(x-y) \, | \rho(x,y) |^2 \, dx \, dy + \right.$$

$$- B_i \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V_i(x-y) \, | \rho_n(x,y) |^2 \, dx \, dy +$$

$$\left. - B_i \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V_i(x-y) \, | \rho_p(x,y) |^2 \, dx \, dy \right\} + \frac{e^2}{4} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} \times$$

$$\times \frac{1}{|x-y|} \left\{ \rho_p(x) \, \rho_p(y) - | \rho_p(x,y) |^2 \right\} dx \, dy + t_0 \int_{\mathbb{R}^3} \rho^{7/3} \, dx \, .$$

where W_i, H_i, M_i, B_i $(i = 1, 2)$ are given constants (which in practice are not independent — roughly speaking $W_i = - B_i$, $H_i = - M_i$) and V_i $(i = 1, 2)$ are given by : $V_i(x) = \exp(- |x|^2/\mu_i^2)$, and $\mu_1, \mu_2 > 0$ are two given constants. Of course, we are using the same notations concerning ρ, ρ_n, ρ_p, τ as in the functional (28) for Skyrme's interaction (section IV).

The HF minimization problem is then

$$I = \operatorname{Inf} \left\{ E(\varphi_1, \ldots, \varphi_A) / \varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \varphi_i \, \varphi_j^* \, dx = \delta_{ij} \right.$$

$$\left. \text{for} \quad 1 \leqslant i,j \leqslant N \quad \text{and for} \quad N+1 \leqslant i,j \leqslant A \right\} . \quad (46)$$

We will not state a result on this problem because exactly the same result as in part iii) of Theorem IV.4 holds here (and the remarks following Theorem IV.1 or Theorem IV.4 also hold here). Of course since $V_i \in L^\infty(\mathbb{R}^3)$ for $i = 1, 2$ the infimum and minimizing sequences are automatically bounded and contrarily to Theorem IV.4 no restrictions on the coefficients need to be made prior to the analysis of minimizing sequences.

VI. SPIN-ORBIT FORCES

Up to now we have constantly ignored the spin dependence of the various wave functions. However, if this omission greatly simplifies the presentation and (probably) the mathematics of the HF minimization problems, for practical and realistic computations one has to cope with the spin dependence and its consequences : the spin-orbit force. It is our goal here to try to explain the form of the spin-orbit force and to show that in order to have a bounded infimum some precautions have to be taken (and it does not seem to have been always the case in the Physics litterature on this matter). Let us also mention that in the remaining sections of this paper, we will again skip the spin dependence even if it can be restored without affecting the mathematical results (provided one considers spin-orbit forces with the appropriate restrictions described below).

First, we explain how wave functions depend on spin and we will do so by only explaining the computational rules. In everything we said in section II, one has to understand now that $\Phi(x_1, \dots, x_A)$, $\varphi_i(x)$ in fact depend on other variables namely

$$\Phi(x_1, \sigma_1 ; x_2, \sigma_2 ; \dots ; x_A, \sigma_A) , \quad \varphi_i(x, \sigma)$$

where the spin variables σ_i take only two values say $+1$ and -1. If we denote by $\bar{x}_i = (x_i, \sigma_i)$ $(1 \leqslant i \leqslant A)$, the Pauli principle now states that the antisymmetry condition (2) has to be understood now as a condition on permutations of the variables $\bar{x}_i (1 \leqslant i \leqslant A)$. Then the remainder of the derivation of HF problems goes through as before. It is possible to consider now $\varphi_i(x, \sigma)$ as a pair of complex-valued functions (spinor) that we will indifferently denote by $(\varphi_i(1), \varphi_i(-1))$ or $(\varphi_i^+, \varphi_i^-)$.

The orthogonality condition becomes (if no differences between neutrons and protons are made)

$$\int_{\mathbb{R}^3} \varphi_i(1) \varphi_j^*(1) + \varphi_i(-1) \varphi_j^*(-1) \, dx = \delta_{ij} , \quad \text{for} \quad 1 \leqslant i, j \leqslant A . \qquad (47)$$

The spin dependence affects the Hamiltonian H and the potential V in two ways : the first one is through the so-called spin-exchange operators (P_σ) which will basically mix the various products of φ_i. The second one is more dramatic; it is the so-called spin-orbit force which can be thought of as an additional two-body term.

Typical models of the spin-orbit force are zero-range models comparable to the choice (5) of potentials. This model leads to a functional $\tilde{E}(\varphi_1, \dots, \varphi_A)$ which in the case of Skyrme's interaction (see section IV) is given by

$$\tilde{E}(\varphi_1, \dots, \varphi_A) = E(\varphi_1, \dots, \varphi_A) + \frac{\beta}{2} \int_{\mathbb{R}^3} | J_n |^2 + | J_p |^2 \, dx + $$
$$+ \frac{W_0}{2} \int_{\mathbb{R}^3} (\nabla \rho, J) + (\nabla \rho_n, J_n) + (\nabla \rho_p, J_p) \, dx \qquad (48)$$

where E is given by (28), the parameter β already occurs in E, W_0 is a positive parameter, J is the so-called spin density that we describe below and J_n, J_p are the spin-densities for the neutrons and protons and are built in the same way as J restricting the various sums to the neutrons or protons wave functions φ_i (as we did for ρ_n, ρ_p ...). Let us also mention that the densities τ, ρ now mean of course

$$\tau = \sum_{i=1}^{A} (|\nabla\varphi_i^+|^2 + |\nabla\varphi_i^-|^2), \quad \rho = \sum_{i=1}^{A} (|\varphi_i^+|^2 + |\varphi_i^-|^2).$$

We now describe J : J is a function $\mathbb{R}^3$ taking values in $\mathbb{R}^3$ which may be written as (see [48])

$$J(x) = (-i) \sum_{j,\sigma,\sigma'} \varphi_j^*(x, \sigma) [\nabla\varphi_j(x, \sigma') \times \langle \sigma | \vec{\sigma} | \sigma' \rangle] \tag{49}$$

where $\vec{\sigma}$ is the Pauli spin matrix. The above bracket means that $\langle \sigma | \vec{\sigma} | \sigma' \rangle$ is a point of $\mathbb{R}^3$ whose coordinates are the results of the action of the 2×2 matrices σ_x, σ_y, σ_z described below on (σ, σ') where the spin variables σ, σ' take values now in $\begin{pmatrix}1\\0\end{pmatrix}$ or $\begin{pmatrix}0\\1\end{pmatrix}$ with the conventions " $+ = \begin{pmatrix}1\\0\end{pmatrix}$ "," $- = \begin{pmatrix}0\\1\end{pmatrix}$ ". The matrices σ_x, σ_y, σ_z are given by

$$\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}, \quad \sigma_y = \begin{pmatrix}0 & i\\-i & 0\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}. \tag{50}$$

For example if $\sigma = \sigma' = \begin{pmatrix}1\\0\end{pmatrix}$ then

$$\langle \sigma | \sigma_x | \sigma' \rangle = (1 \quad 0)\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$$

$$\langle \sigma | \sigma_y | \sigma' \rangle = (1 \quad 0)\begin{pmatrix}0 & i\\-i & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0$$

$$\langle \sigma | \sigma_z | \sigma' \rangle = (1 \quad 0)\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 1$$

and the point $\langle \sigma | \vec{\sigma} | \sigma' \rangle$ is the point $\begin{pmatrix}0\\0\\1\end{pmatrix}$.

In general the above quantity J is not real and at this point we need to explain an important assumption in Hartree-Fock theory in Nuclear Physics. When including spin dependence and spin-orbit forces (as one should), one has to work in the case of even-even nuclei i.e. one assumes that N, Z and so A are even. Furthermore one assumes that the subspace of occupied single-particle states is invariant under time reversal and this means mathematically that for all j ($j \in \{1, \dots, N\}$ or $j \in \{N+1, \dots, A\}$) there exists j' ($j' \in \{1, \dots, N\}$ or $j' \in \{N+1, \dots, A\}$) such that

$$\varphi_{j'}(x, \sigma) = -\sigma\varphi_j^*(x, -\sigma) \quad \text{for all} \quad x \in \mathbb{R}^3, \quad \sigma = \pm 1 \tag{51}$$

i.e. $\varphi_{j'}^+ = -\varphi_j^{-*}$, $\varphi_{j'}^- = \varphi_j^{+*}$.

It is possible to use this assumption by dividing by two the number of unknowns (N, Z, A become $N/2$, $Z/2$, $A/2$) and we still denote by N, Z, A those reduced numbers) : then the HF minimization problem and the functional remain the same and one may compute the three components J_x, J_y, J_z of J. A tedious computation yields

$$J_x = \sum_{i=1}^{A} \{ \mathrm{Im}(\varphi_i^*(1)\nabla_y\varphi_i(1)) - \mathrm{Im}(\varphi_i^*(-1)\nabla_y\varphi_i(-1)) + \\ + \mathrm{Re}(\varphi_i^*(1)\nabla_z\varphi_i(-1)) - \mathrm{Re}(\varphi_i^*(-1)\nabla_z\varphi_i(1)) \} \tag{52}$$

$$J_y = \sum_{i=1}^{A} \{ -\mathrm{Im}(\varphi_i^*(1)\nabla_x\varphi_i(1)) + \mathrm{Im}(\varphi_i^*(-1)\nabla_x\varphi_i(-1)) + \\ + \mathrm{Im}(\varphi_i^*(1)\nabla_z\varphi_i(-1)) + \mathrm{Im}(\varphi_i^*(-1)\nabla_z\varphi_i(1)) \} \tag{53}$$

$$J_z = \sum_{i=1}^{A} \{ -\mathrm{Re}(\varphi_i^*(1)\nabla_x\varphi_i(-1)) + \mathrm{Re}(\varphi_i^*(-1)\nabla_x\varphi_i(1)) + \\ - \mathrm{Im}(\varphi_i^*(1)\nabla_y\varphi_i(-1)) - \mathrm{Im}(\varphi_i^*(-1)\nabla_y\varphi_i(1)) \}. \tag{54}$$

We will only investigate here the difficulties concerning the boundedness of minimizing sequences and the finiteness of the infimum, coming from the addition of the two spin-orbit terms in the functional $\tilde{E}$ given by (48). Of course, we are interested in

$$I = \mathrm{Inf}\left\{ \tilde{E}(\varphi_1, \dots, \varphi_A) \mid \varphi_i \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho\tau \, dx < \infty, \right.$$

$$\sum_{\sigma} \int_{\mathbb{R}^3} \varphi_i(x, \sigma)\, \varphi_j^*(x, \sigma)\, dx = \delta_{ij} \text{ for } 1 \leqslant i, j \leqslant N \text{ and}$$

$$\text{for } N + 1 \leqslant i, j \leqslant A \,\} \tag{55}$$

Once these questions are solved positively, then the analysis of (55) goes along the same lines than in the preceding sections (and raises even more open problems).

The considerations we give below show that I is finite in the case of the Skyrme's interaction if W_0 is small enough (and α, β, δ, γ satisfy the conditions of i) in Theorem IV.4), while for other interactions having finite ranges (but not zero) I is never finite. The conclusion is that the spin-orbit force cannot be taken as a zero-range two-body interaction and one has to use instead spin-orbit force term like

$$e^{-(r_1 - r_2)^2/\mu^2}[(r_1 - r_2) \times (\vec{\nabla}_1 - \vec{\nabla}_2).(\vec{\sigma}_1 + \vec{\sigma}_2)] .$$

We will not try to explain to non-expert readers what this terms means; let us just mention that it leads to HF minimization problems involving terms like the ones we are analyzing except that these terms are nonlocal and so present no more singularities nor unbounded features.

By inspecting the proof of parts i), ii) of Theorem IV.4, one checks easily that part ii) still holds for $\tilde{E}$ and thus we will assume that α, β, δ, γ satisfy the conditions of part i) of Theorem IV.4. Therefore we find that if $(\varphi_1, \ldots, \varphi_A)$ are in the minimizing set

$$\tilde{E}(\varphi_1, \ldots, \varphi_A) \geqslant \nu \int_{\mathbb{R}^3} \tau + \rho\tau \, dx - C + \frac{\beta}{2} \int_{\mathbb{R}^3} |J_n|^2 + |J_p|^2 \, dx + $$
$$+ \frac{W_0}{2} \int_{\mathbb{R}^3} (\nabla\rho, J) + (\nabla\rho_n, J_n) + (\nabla\rho_p, J_p) \, dx$$

for some constants ν, $C > 0$. It follows easily that if W_0 is small ($W_0^2 < 8\,\nu\beta$), I is finite and if $\tilde{E}(\varphi_1, \ldots, \varphi_A) \leqslant R$ then $\int_{\mathbb{R}^3} \tau + \rho\tau \, dx \leqslant C_R$ for some positive constant C_R.

Now, we are going to show by an example that I is no more finite (i.e. $I = -\infty$) if we consider more realistic interactions such as the ones considered in section V. To be more specific, we consider the functional

$$\tilde{E}(\varphi_1, \dots, \varphi_A) = E(\varphi_1, \dots, \varphi_A) + \frac{W_0}{2} \int_{\mathbb{R}^3} (\nabla\rho, J) + (\nabla\rho_n, J_n) + (\nabla\rho_p, J_p)\, dx \tag{56}$$

where E is given by (45). We claim that this functional is not bounded from below on the minimizing set $\left\{ \varphi_i \in H^1(\mathbb{R}^3), \sum \int_{\mathbb{R}^3} \varphi_i\, \varphi_j^*\, dx = \delta_{ij}, 1 \leqslant i, j \leqslant N, N+1 \leqslant i, j \leqslant A \right\}$.

In fact, we believe that related examples show that even in the case when E is given by (48) $I = -\infty$ if W_0 is not small enough. This claim is shown at the end of this section by another example. To prove our claim, we begin by a simple scaling argument where $\lambda > 0$ is the scaling parameter $(\varphi_1, \dots, \varphi_6)$ is any test function in the minimizing set

$$\tilde{E}\left[\lambda^{-3/2}\, \varphi_1\left(\frac{\cdot}{\lambda}\right), \dots, \lambda^{-3/2}\, \varphi_A\left(\frac{\cdot}{\lambda}\right)\right] = \frac{1}{\lambda^2}\left[\frac{\hbar^2}{2m} \int_{\mathbb{R}^3} \tau\, dx\right] + C_\lambda + $$
$$+ \frac{1}{\lambda} \frac{e^2}{4} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} \frac{1}{|x-y|} \{ \rho_p(x)\, \rho_p(y) - |\rho_p(x,y)|^2 \}\, dx\, dy$$
$$+ \frac{t_0}{\lambda^4} \int_{\mathbb{R}^3} \rho^{7/3}\, dx + \frac{1}{\lambda^5} \frac{W_0}{2} \int_{\mathbb{R}^3} (\nabla\rho, J) + (\nabla\rho_n, J_n) + (\nabla\rho_p, J_p)\, dx$$

where C_λ is a bounded constant (depending on $\varphi_1, \dots, \varphi_A$). The example below shows that the last term may be negative and thus our claim is proved sending λ to 0. As in the proof of Theorem IV.4 it is enough to build $\varphi_1, \dots, \varphi_A$ near 0 and we will actually build $\varphi_1, \dots, \varphi_A$ so that τ, ρ, ρ^q (for $q < 9$), $|\nabla\rho|^2$ are integrable near 0 while $\rho(\operatorname{div} J)$ has constant sign and is not integrable at 0. Then it is easy to approximate and obtain values which go to $-\infty$. Our choice of $\varphi_1, \dots, \varphi_A$ is the following : for $i \geqslant 3$ take φ_i to be 0 near 0, for $i \leqslant 2$ take φ_i^- to be 0 near 0 and φ_2^+ real near 0. Denote by $\varphi = \varphi_2^+$, $\varphi_1^+ = \psi_1 + i\psi_2$ where φ, ψ_1, ψ_2 are real. We find that

$$\frac{W_0}{2} \int_{\mathbb{R}^3} (\nabla\rho, J)\, dx = -\frac{W_0}{2} \int_{\mathbb{R}^3} \rho \operatorname{div} J\, dx$$

and nearby 0, div J reduces to $2\,\mathrm{Im}\left(\frac{\partial}{\partial x_1}\psi^*\frac{\partial}{\partial x_2}\psi\right)$. Observe also that the term in ρ div J given by

$$\int_{\mathbb{R}^3}(\psi_1^2+\psi_2^2)\left(\frac{\partial}{\partial x_2}\psi_1\frac{\partial}{\partial x_1}\psi_2-\frac{\partial}{\partial x_1}\psi_2\frac{\partial}{\partial x_2}\psi_1\right)dx=0\,.$$

Hence, we only have to look at $\Psi=\varphi^2\left(\frac{\partial}{\partial x_1}\psi_1\frac{\partial}{\partial x_2}\psi_2-\frac{\partial}{\partial x_1}\psi_2\frac{\partial}{\partial x_2}\psi_1\right)$ near 0. We next choose $\varphi(x)=|x|^\alpha$ near 0 for some $\alpha<0$ to be determined later on, and we take $\psi_1(x)=\zeta(x)\cos\theta(x)$, $\psi_2(x)=\zeta(x)\sin\theta(x)$. So $\Psi(x)=|x^2|^\alpha\zeta(x)\left(\frac{\partial}{\partial x_1}\zeta\frac{\partial}{\partial x_2}\theta-\frac{\partial}{\partial x_1}\theta\frac{\partial}{\partial x_2}\zeta\right)$. We finally choose $\zeta(x)=(x_1^2+bx_2^2+x_3^2)^{\beta/2}$, $\theta(x)=|x|^{\gamma/2}$ with $b>0$, $b\neq1$ and the exponents β, γ will be determined later on. With these choices Ψ is given by $\Psi=\beta\gamma r^\alpha s^\beta x_1x_2(1-b)\times s^{\beta-2}r^{\gamma-2}$ where $s=(x_1^2+bx_2^2+x_3^2)^{1/2}$. Therefore Ψ is not integrable at 0 if $2\alpha+2\beta+\gamma\leqslant-1$; while τ, ρ, ρ^q (for $q>1$), $|\nabla\rho|^2$ are integrable if $\alpha>-1/4$, $\beta>-1/4$, $\alpha>-3/(2q)$, $\beta>-3/(2q)$, $\beta+\gamma>-1/2$. Then if $q<9$ choose $\alpha,\beta<-\frac{1}{6}$ near $-\frac{1}{6}$, $\gamma<-\frac{1}{3}$ near $-\frac{1}{3}$ then all the above conditions are satisfied.

We would like to conclude this section by inspecting the size of the spin-orbit term $\frac{W_0}{2}\int_{\mathbb{R}^3}\nabla\rho.J\,dx$ in the case of a spherically symmetric configuration (the precise meaning of that choice will be given in section VIII). Following Vautherin and Brink [48] we see that

$$J=\frac{x}{|x|}\bar{J}(|x|)\,,$$

$$\bar{J}=\frac{1}{4\pi r^3}\sum_\alpha(2j_\alpha+1)\left[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)-\frac{3}{4}\right]R_\alpha^2(|x|)$$

while $\rho(x)=\frac{1}{4\pi r^2}\sum_\alpha(2j_\alpha+1)R_\alpha^2(|x|)$; where l_α is some positive integer, $j_\alpha=l_\alpha\pm\frac{1}{2}$ and the sum over α means the so-called sum over occupied states (the set of levels compatible with the numbers of nucleons..., see section VIII).

Hence, the spin-orbit term gives

$$\frac{W_0}{2}\int_{\mathbb{R}^3} \nabla\rho . J\, dx = W_0 \int_0^\infty \left\{ \sum_\alpha (2 j_\alpha + 1) \left[R_\alpha R'_\alpha - \frac{1}{r} R_\alpha^2 \right] \right\} \cdot \frac{1}{4\pi r^3} \times$$

$$\times \left\{ \sum_\beta (2 j_\beta + 1) \left[j_\beta(j_\beta + 1) - l_\beta(l_\beta + 1) - \frac{3}{4} \right] R_\beta^2 \right\} dr .$$

If we choose only one occupied state α (this may always be achieved by taking various R_α with distinct supports in $(0, \infty)$) with $j_\alpha = l_\alpha + \frac{1}{2}$, we deduce

$$\frac{W_0}{2}\int_{\mathbb{R}^3} \nabla\rho . J\, dx = \frac{W_0}{4\pi}(2 j_\alpha + 1)^2 l_\alpha \int_0^\infty \left[R_\alpha^3 R'_\alpha - \frac{1}{r} R_\alpha^4 \right] \frac{1}{r^3} dr =$$

$$= - \frac{W_0}{4\pi}(2 j_\alpha + 1)^2 l_\alpha \left(\frac{1}{4} \int_0^\infty R_\alpha^4 \frac{1}{r^4} dr \right) .$$

And the above scaling argument shows that even in the context of spherically symmetric configurations, the spin-orbit term is " too unbounded ". In fact, the above computation also shows that even for Skyrme's interaction conditions on W_0^2 (compared to the other constants β, α...) have to be imposed in order to have a meaningful HF minimization problem.

VII. A-BODY PROBLEMS IN NUCLEAR PHYSICS AND THOMAS-FERMI APPROXIMATIONS

In this section, we first make a few comments on the translation-invariant A-body problems of the form (1) and on the minimization problem (8). Then we investigate the role of the density-dependent term in the Hamiltonians H which are being used in practice in Nuclear Physics. Finally, we conclude this section by discussion the validity of HF approximation and we briefly discuss the Thomas-Fermi approximation.

We begin with problem (8) where H is given by (1). In the remarks which follow we will not bother to give precise assumptions on V which guarantee an easy justification of the arguments below (again it is an easy exercise that we leave to the reader). We first observe that (8) has never a minimum : indeed, let $\Phi \in \mathcal{H}$ with $\int_{\mathbb{R}^3} |\Phi|^2 dx = 1$ we consider for $\lambda > 0$

$$\Phi_\lambda(x_1, \ldots, x_A) = \frac{1}{\sqrt{\lambda}} \Phi\left(x_1 - \bar{x} + \frac{1}{\lambda}\bar{x}, \ldots, x_n - \bar{x} + \frac{1}{\lambda}\bar{x} \right) \qquad (57)$$

where $\bar{x} = \frac{1}{A} \sum_{i=1}^{A} x_i$. One checks easily that $\Phi_\lambda \in \mathscr{H}$ and $\int_{\mathbb{R}^{3A}} |\Phi_\lambda|^2 \, dx = 1$. Next we compute $\mathscr{E}(\Phi_\lambda) = (H\Phi_\lambda, \Phi_\lambda)_{L^2}$ and we obtain

$$\mathscr{E}(\Phi_\lambda) = \mathscr{E}(\Phi) + \frac{\hbar^2}{2m} \frac{1}{A} \left(\frac{1}{\lambda^2} - 1 \right) \int_{\mathbb{R}^{3A}} \left| \sum_i \nabla_i \Phi \right|^2 dx .$$

Hence, if Φ is a minimum of (8) the above equality implies $\sum_i \nabla_i \Phi = 0$ and this is not possible since $\Phi \in L^2$, $\Phi \not\equiv 0$.

The above equality also shows that the ground state energy E is also given by

$$E = \operatorname{Inf} \left\{ \frac{\hbar^2}{2m} \sum_i \int_{\mathbb{R}^{3A}} |\nabla_i \Phi|^2 \, dx - \frac{\hbar^2}{2mA} \int_{\mathbb{R}^{3A}} \left| \sum_i \nabla_i \Phi \right|^2 dx + \right.$$
$$\left. + \sum_{i<j} \int_{\mathbb{R}^{3A}} V(x_i - x_j) \, |\Phi|^2 \, dx / \Phi \in \mathscr{H} \cap H^1(\mathbb{R}^{3A}), \int_{\mathbb{R}^{3A}} |\Phi|^2 \, dx = 1 \right\}.$$

And now the translation invariance does not imply anymore a priori that minima do not exist. In fact to our knowledge no existence results of minima for $A \geqslant 3$ are known for the above problem. Observe also that the above quadratic functional is invariant under the transformation $(\Phi \to \Phi_\lambda)$ for $\lambda > 0$.

In fact, in practice it may be important to apply HF method to the above functional instead of $(H\Phi, \Phi)$ and when we inject Slater determinants into the above functional we obtain the following quantity (which clearly replaces the term $\frac{\hbar^2}{2m} \int_{\mathbb{R}^3} \tau \, dx$ that we had in the preceding sections)

$$\frac{\hbar^2}{2m} \left(1 - \frac{1}{A} \right) \int_{\mathbb{R}^3} \tau \, dx + \frac{\hbar^2}{2m} \frac{2}{A} \sum_{i<j} \left| \int_{\mathbb{R}^3} \nabla \varphi_i \, \varphi_j^* \, dx \right|^2 \tag{59}$$

and everything we did in the preceding sections is easily adapted to this new situation.

We now make two remarks for improving the Physics applications of HF methods. First of all, there is a slight difference of mass between neutrons and protons and this could be incorporated in H and in everything we did before by replacing $-\frac{\hbar^2}{2m} \sum_{i=1}^{A} \Delta_{x_i}$ by $-\frac{\hbar^2}{2m_n} \sum_{i=1}^{N} \Delta_{x_i} - \frac{\hbar^2}{2m_p} \sum_{i=N+1} \Delta_{x_i}$ where m_n, m_p denote respectively the masses of neutrons and protons.

The next remark concerns the density dependent terms : in the preceding sections (III to VI) all HF functionals incorporated terms nonlinear with ρ

homogeneous of a degree different from 4 and obviously such terms cannot be obtained through the method presented in section II. In fact, to improve the numerical computations obtained through HF methods Nuclear physicists have added to the Hamiltonian H phenomenological terms of the form

$$t_3 \sum_{i<j<k} V(x_i - x_j)\, V(x_j - x_k) \tag{60}$$

where V for example may be $V = \delta_0$. Now if we use Slater determinants this term gives some term like

$$\frac{1}{6} t_3 \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} \rho(x)\, V(x-y)\, \rho(y)\, V(y-z)\, \rho(z)\, dx\, dy\, dz$$

or $\frac{1}{6} t_3 \int_{\mathbb{R}^3} \rho^3\, dx$ if $V = \delta_0$. Recalling that we are suppressing the spin dependence one sees that such a term is equivalent on Slater determinants to a two-body density-dependent interaction

$$\frac{1}{3} t_3\, \rho\left(\frac{x_i + x_j}{2}\right) \delta(x_i - x_j) \tag{61}$$

(all this is formal because the absence of spin does make matters a bit trivial). Roughly speaking the term (60) provides a simple phenomenological representation of many-body effects and is supposed to describe the influence of all other nucleons to the interaction between two of them. It has also been observed that instead of ρ it is often better to consider $\rho^{2/3}$ (see H. Bethe [8]) which leads to the term $\int_{\mathbb{R}^3} \rho^{2+2/3}\, dx$ used in section V.

We now conclude this section by examining the validity of HF approximations to (8). In [31], E. H. Lieb and B. Simon proved (at least for Coulombic systems) that the ground state energy E^A given by (8) and its HF approximation E^A_{HF} given by (11) have similar asymptotic behaviours as A go to $+\infty$. More precisely one has for general classes of V

$$\frac{E^A}{A^{7/3}}, \quad \frac{E^A_{\mathrm{HF}}}{A^{7/3}} \underset{A \to \infty}{\to} E_{\mathrm{TF}} \tag{62}$$

where E_{TF} is the infimum of the so-called Thomas-Fermi approximation of (8)

$$E_{\mathrm{TF}} = \mathrm{Inf}\left\{ \frac{3\gamma}{5} \int_{\mathbb{R}^3} \rho^{5/3}\, dx + \frac{1}{2} \int_{\mathbb{R}^3} \times \int_{\mathbb{R}^3} \rho(x)\, V(x-y)\, \rho(y)\, dx\, dy / \rho \in \right.$$

$$\in L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3), \quad \rho \geqslant 0 \text{ a.e.} \int_{\mathbb{R}^3} \rho \, dx = 1 \Big\} \quad (63)$$

where γ is given by $(6\,\pi^2)^{2/3}\dfrac{\hbar^2}{2\,m}$. These results were first proved by E. H. Lieb and B. Simon [31] and the original proof was later simplified by B. Baumgartner [4], E. H. Lieb [26], [27] : an inspection of the proof (confirmed to the second author by E. H. Lieb) shows that the result holds for general V. In fact, in Nuclear Physics it is expected that $\dfrac{E_{\text{HF}}^A}{A} \underset{A\to\infty}{\to} C_0 < 0$ (volume energy constant) : this means that for realistic V $E_{\text{TF}} = 0$. Furthermore, defining E_{TF}^A by (63) where $\int_{\mathbb{R}^3} \rho\, dx = 1$ is replaced by $\int_{\mathbb{R}^3} \rho\, dx = A$ one would like to prove that $\dfrac{E^A}{A}, \dfrac{E_{\text{HF}}^A}{A}, \dfrac{E_{\text{TF}}^A}{A} \underset{A\to\infty}{\to} C_0$. Of course if $E_{\text{TF}} < 0$, then one deduces from (62) that $E^A/E_{\text{HF}}^A \underset{A\to\infty}{\to} 1$.

Concerning the TF minimization problems (63), let us mention the references [36], [33] where related problems are treated. Applying the method in [33], we find that if V is given by (5) $E_{\text{TF}} = 0$ and there is no minimum while if V is given by (3) or (4) the concentration-compactness argument applies. And it is shown in [33] that every minimizing sequence is relatively compact up to a translation if and only if $E_{\text{TF}} < 0$. In particular if $E_{\text{TF}} < 0$, there exists a minimum and if $\alpha, \beta < 0$ then this minimum is spherically symmetric, nonincreasing with respect to $|x|$. Finally, one checks easily that if $\alpha^- + \beta^-$ is small then $E_{\text{TF}} = 0$ while if α, β are negative and large $E_{\text{TF}} < 0$.

VIII. SOLUTIONS WITH SYMMETRIES OF HARTREE-FOCK EQUATIONS

All the minimization problems we considered in the preceding sections are invariant under orthogonal transformations of $\mathbb{R}^3$: if R is an orthogonal matrix then denoting by $\tilde{\varphi}_i(.) = \varphi_i(R.)$ for all i we check immediately that

$$E(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_A) = E(\varphi_1, \ldots, \varphi_A)$$

for all the functionals we considered previously, while the orthogonality conditions (10) still hold for $(\tilde{\varphi}_1, \ldots, \tilde{\varphi}_A)$.

It is thus natural to look for solutions of the HF equations with certain invariance properties by a subgroup of the group of orthogonal transforms of $\mathbb{R}^3$. For instance one may look for solutions with spherical symmetry or cylindrical symmetry and in particular one may study the same HF minimization problems with the additional constraint of invariance by a chosen subgroup But of course there are various ways to impose spherical symmetry on $(\varphi_1, \ , \varphi_A)$ (or cylindrical symmetry) One possibility is to impose that all φ_i are spherically symmetric i e φ_i only depend on $|x|$ However this is not really satisfactory from the Physics view point since, even when solutions with such symmetries exist (and this is not always the case in view of numerical experiments), in general such a solution gives a value to the functional which is too high to yield any information on problems like (8)

To explain the meaning of spherically symmetric solutions in Nuclear Physics we take an example namely the case of the functional (28) and to simplify we assume that $e = 0$ so we consider

$$E(\varphi_1, \ , \varphi_A) = \int_{\mathbb{R}^3} \left\{ \frac{\hbar^2}{2m} - \frac{t_0}{2}\left[\left(1 + \frac{x_0}{2}\right)\rho^2 - \left(x_0 + \frac{1}{2}\right)(\rho_n^2 + \rho_p^2)\right] + \right.$$

$$+ \frac{\alpha}{4}\rho\tau - \frac{\beta}{4}(\rho_n\tau_n + \rho_p\tau_p) + \frac{\gamma}{16}|\nabla\rho|^2 - \frac{\delta}{16}(|\nabla\rho_n|^2 + |\nabla\rho_p|^2) +$$

$$\left. + \frac{t_3}{3}\rho\rho_n\rho_p \right\} dx$$

Recall that we work with the following orthogonality conditions

$$\int_{\mathbb{R}^3} \varphi_i \varphi_j^* \, dx = \delta_{ij} \quad \text{for} \quad 1 \leqslant i, j \leqslant N \quad \text{and for} \quad N + 1 \leqslant i, j \leqslant A \tag{65}$$

Now if we assume there exists a critical point of E given by (64) with the constraints (65) such that ρ_n, ρ_p, τ_n, τ_p are spherically symmetric then up to some unitary transform of the form (29) the HF equations may be written as

$$- \operatorname{div}\left(\frac{\hbar^2}{2\, m_q^*(r)}\nabla\varphi_i\right) + V_q(r)\,\varphi_i = e_i\,\varphi_i \quad \text{on} \quad \mathbb{R}^3 \tag{66}$$

where $e_1, \ , e_A$ are the Lagrange multipliers, $q = n$ if $1 \leqslant i \leqslant N$, $q = p$ if $N + 1 \leqslant i \leqslant A$, $r = |x|$ and m_n^*, m_p^*, V_n, V_p are spherically symmetric functions which are easily computed from the expression of E (64) The quantities m_q^* are often called effective masses It is well-known that φ_i being an eigenfunction of the elliptic operator L_q given by $\left\{ - \operatorname{div}\left(\frac{\hbar^2}{2\, m_q^*(r)}\nabla\right) + V_q \right\}$ must be a product of a function $\phi_i(r)$ by a spherical harmonic ψ_i i e an eigenfunction of the Laplace-Beltrami operator $(-\Delta_S)$ on the sphere S^2 of $\mathbb{R}^3$ But then the orthogonality conditions (65) imply that if for some $i \in \{1, \ , N\}$ (for example)

$\varphi_i = \phi_i(r)\,\psi_i(\theta)$ and $-\Delta_S\psi_i = E_i\,\psi_i$ then denoting by m the multiplicity of the eigenvalue E_i there exist $(m-1)$ indices in $\{1, \ldots, N\}$ distinct from i for which the associated ψ is also an eigenfunction of $-\Delta_S$ with the eigenvalue E_i. In other words N (and Z) splits into the sum of say k multiplicities of eigenvalues of $(-\Delta_S)$ and the angular functions ψ_i associated to φ_i span the eigenspaces of these eigenvalues. In view of the increasing multiplicity of eigenvalues of $(-\Delta_S)$ as they increase, it is easy to see that for given N and Z they are only a finite number of choices for the angular dependences of the functions φ_i. This decomposition is precisely the meaning of a spherically symmetric solution for HF equation.

Of course, we could minimize E imposing (65) and the above formulation of spherical symmetry but it is somewhat simpler (and better for the values of E we get this way a priori) to consider instead

$$I^S = \operatorname{Inf}\left\{ E(\varphi_1, \ldots, \varphi_A)/\varphi_i \in H^1(\mathbb{R}^3) \quad \text{for} \quad 1 \leqslant i \leqslant A, (65) \text{ holds}, \right.$$
$$\left. \int_{\mathbb{R}^3} \rho\tau\, dx < \infty,\ \rho_n, \rho_p, \tau_n, \tau_p \text{ are spherically symmetric} \right\}. \quad (67)$$

Observe nevertheless that if we find a minimum of (67) then by the above arguments the minimum is really of the form we described above so there is no loss of generality by considering the minimizing set described in (67).

And one proves easily the following result using either the concentration-compactness arguments with symmetry ([34]) or the simpler fact that if ρ^m is bounded in $L^1(\mathbb{R}^3) \cap H^1(\mathbb{R}^3)$ and is spherically symmetric then ρ^m is compact in $L^p(\mathbb{R}^3)$ for $1 < p < 6$ (see W. Strauss [46], H. Berestycki and P. L. Lions [5], P. L. Lions [37]). Before stating the result we just need a notation

$$I^s(m_1, \ldots, m_A) = \operatorname{Inf}\left\{ E(\varphi_1, \ldots, \varphi_A)/\varphi_i \in H^1(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \rho\tau\, dx < \infty, \right.$$
$$\int_{\mathbb{R}^3} \varphi_i\,\varphi_j^*\, dx = m_i\,\delta_{ij} \text{ for } 1 \leqslant i, j \geqslant N,\ N+1 \leqslant i, j \leqslant A,$$
$$\left. \rho_n, \rho_p, \tau_n, \tau_p \text{ are spherically symmetric} \right\} \quad (68)$$

where $m_i \geqslant 0$ for all $i \in \{1, \ldots, A\}$.

THEOREM VIII.1 : *Assume that* $\alpha > (\beta + \delta)/2$, $\alpha + \delta \wedge \gamma > \delta + \beta$. *Then, every minimizing sequence of* (67) *is relatively compact in* $H^1(\mathbb{R}^3)$ (*and* $\rho\tau$ *is* *relatively compact in* $L^1(\mathbb{R}^3)$) *if and only if the following conditions holds*

$$I^S < I^S(m_1, \ldots, m_A)\,, \quad \text{for all} \quad m_i \in [0, 1]\,(1 \leqslant i \leqslant A)$$
$$\text{such that } \sum_{i=1}^{A} m_i < A\,. \qquad (69)$$

In particular there exists a minimum of (67) *if* (69) *holds.*

Remarks : 1) As in many results above, the condition (69) seems difficult to check for $A \leqslant 2$ and in fact numerical computations that the existence of a minimum is highly dependent on A.

2) Again it is possible to treat the case when $\hbar = 0$. ∎

For realistic interactions and HF problems (thus including spin-orbit forces) the spherical symmetry is imposed by considering $(\varphi_1, \ldots, \varphi_A)$ such that ρ_n, ρ_p, τ_n, τ_p are spherically symmetric; $\rho_n(x, y)$, $\rho_p(x, y)$ satisfy $\rho_q(Rx, Ry) = \rho(x, y)$ for all rotations R of $\mathbb{R}^3$ and for all $q = n, p$; and J_n, J_p have the form

$$J_q(x) = \frac{x}{r} \mid J_q \mid (r)\,,$$

and with these constraints similar results hold.

As we already explained above two arguments may be invoked to prove the analogues of Theorem VIII.1 in the case of more realistic interactions $V(x - y)$. Either one applies the general arguments of P. L. Lions [34] (concentration-compactness principle in presence of symmetries), or one may use more standard compactness arguments due to spherical symmetry as mentioned above. In the latter case however one needs to explain how to pass to the limit on the term

$$\int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V(x - y) \mid \rho_m(x, y) \mid^2 dx\, dy$$

where ρ_m is the density corresponding to a minimizing sequence $(\varphi_1^m, \ldots, \varphi_A^m)$ (thus bounded in $H^1(\mathbb{R}^3)$). We thus assume we have spherically symmetric configurations i.e.

$$\rho_m(Rx, Ry) = \rho_m(x, y) \qquad \forall x, y \in \mathbb{R}^3$$

for all rotations R of $\mathbb{R}^3$. Since V decays at infinity it is enough to explain why, for all $R < \infty$, $\mid \rho_m(x, y) \mid^2 1_{|x-y| \leqslant R}$ is compact in $L^1(\mathbb{R}^3 \times \mathbb{R}^3)$. We then introduce

$$\zeta_m(x) = \int_{|x-y|\leqslant R} |\rho_m(x,y)|^2\, dy$$

which is spherically symmetric ($\zeta_m(Rx) = \zeta_m(x)$). And ζ_m is bounded in $W^{1,1}(\mathbb{R}^3)$ by the definition of ρ and the H^1 bounds on φ_i^m. By P. L. Lions [37], we see that $\zeta_m(x) \leqslant \dfrac{C}{|x|^2}$ on $\mathbb{R}^3$. Therefore, if we prove that $\zeta_m^{1/2}$ is bounded in $L^1(\mathbb{R}^3)$, it is then easy to conclude that ζ_m is compact in $L^1(\mathbb{R}^3)$. But

$$\begin{aligned}
\int_{\mathbb{R}^3} \zeta_m^{1/2}\, dx &\leqslant C \int_{\mathbb{R}^3} \left(\sum_i \int_{|x-y|\leqslant R} |\varphi_i^m(x)|^2 \, |\varphi_i^m(y)|^2\, dy \right)^{1/2} dx \\
&\leqslant C \int_{\mathbb{R}^3} \sum_i \left(\int_{|x-y|\leqslant R} |\varphi_i^m(x)|^2 \, |\varphi_i^m(y)|^2\, dy \right)^{1/2} dx \\
&\leqslant C \sum_i \int_{\mathbb{R}^3} |\varphi_i^m(x)| \left(\int_{|x-y|\leqslant R} |\varphi_i^m(y)|^2\, dy \right)^{1/2} dx \\
&\leqslant C \sum_i \left(\int_{\mathbb{R}^3} |\varphi_i^m(x)|^2\, dx \right)^{1/2} \left(\int_{\mathbb{R}^3} \left(\int_{|x-y|\leqslant R} |\varphi_i^m(y)|^2\, dy \right) dx \right)^{1/2} \\
&\leqslant CA(4\pi R^3)^{1/2},
\end{aligned}$$

for various constants $C \geqslant 0$ and we conclude.

We now conclude this section by a brief discussion of cylindrical symmetric solutions. Let us denote by $s = (x_1^2 + x_2^2)^{1/2}$, $z = x_3$ if $x = (x_1, x_2, x_3)$ is a generic point of $\mathbb{R}^3$. Arguments similar to those given above lead to the following problem

$$I^c = \operatorname{Inf} \left\{ E(\varphi_1, \dots, \varphi_A)/\varphi_i \in H^1(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \rho\tau\, dx < \infty, \right.$$
$$\left. (65) \text{ holds, } \rho_n, \rho_p, \tau_n, \tau_p \text{ are functions of } s, z \text{ only} \right\}, \quad (70)$$

that we extend in the following class of problems

$$I^c(m_1, \dots, m_A) = \operatorname{Inf} \left\{ E(\varphi_1, \dots, \varphi_A)/\varphi_i \in H^1(\mathbb{R}^3); \right.$$
$$\int_{\mathbb{R}^3} \varphi_i \varphi_j^*\, dx = m_i \delta_{ij} \quad \text{for} \quad 1 \leqslant i,j \leqslant N, \quad N+1 \leqslant 1,j \leqslant A; \quad (71)$$

$$\int_{\mathbb{R}^3} \rho\tau\, dx < \infty ; \; \rho_n, \rho_p, \tau_n, \tau_p \text{ are functions of } s, z \text{ only} \Big\}, \tag{71}$$

where $m_1, \ldots, m_A$ are nonnegative constants.

Again, applying the concentration-compactness arguments we see that if $\alpha > (\beta + \delta)/2, \alpha + \delta \wedge \gamma > \delta + \beta$, then every minimizing sequence of (70) is relatively compact up to a translation in z if and only if the following holds

$$I^c < I^c(m_1, \ldots, m_A) + I^c(1 - m_1, \ldots, 1 - m_A) \quad \text{for all} \quad m_i \in [0, 1]$$
$$(1 \leqslant i \leqslant A) \quad \text{such that} \quad \sum_{i=1}^{A} m_i \in (0, A) \tag{72}$$

and there exists a minimum of (70) if (72) holds.

IX. THE SHAPE OF THE NUCLEUS AND SYMMETRY BREAKINGS

Admitting that the HF approximation is valid, then the ground state of a nucleus is supposed to be described by the minima of the various HF minimization problems studied in sections III-VI. In particular the shape of the nucleus will be determined by the density ρ : the nucleus is spherical if ρ is spherically symmetric, or more generally has the symmetries that ρ possesses.

If we keep the notations of the preceding section, we see that the spherical symmetry is broken if $I^s > I$ but it may happen that $I^s > I^c = I$ in which case the spherical symmetry is broken but the minimum (if it exists) still preserves the cylindrical symmetry. While if $I^s \geqslant I^c > I$ then even the cylindrical symmetry is broken. All these phenomena (and many others related to more elaborate symmetries) are known to occur in Nuclear Physics and are very important. The mechanism behind these symmetry breakings is not at all understood neither from the Physics viewpoint nor from the mathematical viewpoint.

We propose here some vague explanations for some of these symmetry breakings and we consider as examples various simpler model problems which could help understanding these phenomena. Before going into these examples, we would like to comment on the physical meaning and implications of such deformed HF ground states. Since the original Hamiltonian is rotationally invariant we know that the real ground state should have a " good total angular momentum ". This aspect which, at first sight, seems to be a defect of HF theory hides, on the contrary, very nice features as briefly explained in the following. In order to restore the symmetry the HF solution is reinterpreted as an intrinsic state capable of rotating into itself. The quantization of such collective rotational motion, achieved by A. Bohr [11] a long time ago leads, to a model predicting excited states whose spectrum should obey the simple law : $E_I = \frac{\hbar^2}{2g} I(I+1)$ where I is the total angular momentum and g is the inertia momentum. Such typical rotational spectra are exhibited by several nuclei (^{152,154}Sm, ^{154}Gd, ^{168}Er) and the HF theory do predict in their cases a deformed intrinsic structure. It must be pointed out that such interpretation of broken symmetries in terms of collective modes is currently used in various branches of modern physics (see J. Goldstone modes [22], Higgs modes in non Abelian Gauge theory [24]). Thus, it appears that the HF method is a much more powerful tool than it looks a priori from a strict mathematical viewpoint.

We begin with a very simple example.

Example 1 : Let B be a ball centered at 0 in $\mathbb{R}^3$. We consider the minimization problem

$$\operatorname{Inf}\left\{ \sum_{i=1}^{A} \int_B |\nabla u_i|^2\, dx - \int_B f\left(\sum_{i=1}^{A} u_i^2\right) dx / u_i \in H_0^1(B) \right.$$

$$\left. \text{for all} \quad 1 \leqslant i \leqslant A\,, \quad \int_B u_i\, u_j\, dx = \delta_{ij} \quad \text{for} \quad 1 \leqslant i,j \leqslant A \right\} \tag{73}$$

where $\lambda > 0$ is a parameter, $u_i\,(1 \leqslant i \leqslant A)$ are real-valued functions, f is a continuous function on $\mathbb{R}^+$ satisfying for example

$$\lim_{t \to +\infty} f(t)\, t^{-5/3} \leqslant 0\,. \tag{74}$$

We claim that <u>if $A = 2$ or if $A = 3$</u> then for λ small the density $\rho = \sum_{i=1}^{A} u_i^2$ is not spherically symmetric where $(u_1, \ldots, u_A)$ is any minimum of the above minimization problem. (The existence of minima is a standard exercise in functional analysis since we are dealing with a bounded domain B and the nonlinearity satisfies some appropriate growth condition.) To prove this claim, we denote by $E(\lambda)$ the value of the above infimum and we observe that for $\lambda = 0$, $E(0)$ is nothing but the sum of the first A eigenvalues of the operator $-\Delta$ in $H_0^1(B)$ and that the corresponding minima for $A = 2$ or 3 are such that ρ is not spherically symmetric. To conclude we just have to prove that $E(\lambda)$ converges to $E(0)$ and that minima $(u_1^\lambda, \ldots, u_A^\lambda)$ of $E(\lambda)$ converge (extracting enough subsequences) to the minima of $E(0)$. Indeed, observe that

$$E(\lambda) \leqslant E(0) + C\lambda, \quad \text{for some} \quad C \geqslant 0$$

while (74) implies easily that for some $C \geqslant 0$

$$\sum_{i=1}^{A} \int_B |\nabla u_i|^2 \, dx + \lambda \int_B f^-(\rho^\lambda) \, dx \leqslant C$$

$$\lambda \int_B f^+(\rho^\lambda) \, dx \underset{\lambda \to 0}{\to} 0 .$$

This yields on one hand that $E(\lambda) \underset{\lambda \to 0}{\to} E(0)$ and on the other hand that if u_i^λ $(1 \leqslant i \leqslant A)$ converge weakly in $H_0(B)$ to u_i then

$$\begin{aligned} \sum_{i=1}^{A} \int_B |\nabla u_i|^2 \, dx &\leqslant \varliminf_{\lambda \to 0} \sum_{i=1}^{A} \int_B |\nabla u_i^\lambda|^2 \, dx \\ &\leqslant \varliminf_{\lambda \to 0} \left\{ \sum_{i=1}^{A} \int_B |\nabla u_i^\lambda|^2 \, dx + \lambda \int_B f^-(\rho^\lambda) \, dx \right\} \\ &\leqslant \lim_{\lambda \to 0} E(\lambda) = E(0) \end{aligned}$$

and since the constraints pass to the limit, our claim is proved.

One sees what is the mechanism involved in the above example and it seems that this mechanism plays a role in Nuclear Physics : roughly speaking it is expected that symmetry breakings " have more chances to occur " for those A such that the combinatorics of filling our Slater determinants with spherical harmonics (as we explained in the preceding section) do not make possible the use of only the lowest possible eigenvalues (or energy levels) of $(-\Delta_s)$. This explanation is very much related to what are called in Physics magical numbers. Of course, this tentative explanation has to be confirmed or infirmed by the examination of more realistic problems than (73). We propose another model problem for which it would already be interesting to decide whether there is symmetry breaking or not. We will only mention the case $A = 2$.

Example 2 : We consider now

$$I(1, 1) = \operatorname{Inf} \left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + |\nabla v|^2 \, dx - \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} u^2(x) \, V(x - y) \, v^2(y) \, dx \, dy \right.$$
$$\left. u, v \in H^1(\mathbb{R}^3) , \quad \int_{\mathbb{R}^3} u^2 \, dx = \int_{\mathbb{R}^3} v^2 \, dx = 1 \right\} \quad (75)$$

where $\lambda > 0$ and V is spherically symmetric and satisfies $V = V_1 + V_2$ where

$V \in L^{p_i}(\mathbb{R}^3)$ $(i = 1, 2)$ for some $p_i \in \left[\frac{3}{2}, \infty\right)$. The main difference between (75) and HF problems is the fact that we do not assume anymore that $\int_{\mathbb{R}^3} uv\, dx = 0$ and it is possible that this type of constraints plays an important role in symmetry breakings. We prove below that as soon as $I(1, 1) < 0$ all minimizing sequences are relatively compact in $H^1(\mathbb{R}^3)$ up to a translation and thus there exists a minimum of (75). By symmetrization techniques minima are spherically symmetric if V is nonnegative, nonincreasing with respect to $|x|$. The case when V does not have these properties is totally open and this is the interesting case for Nuclear Physics.

To prove the above claim, we have to show (using the concentration-compactness method) that if $I(1, 1) < 0$ then

$$I(1, 1) < I(\lambda, \mu) + I(1 - \lambda, 1 - \mu) \text{ for } 0 \leqslant \lambda \leqslant 1\,,\ 0 \leqslant \mu \leqslant 1 \text{ and } 0 < \lambda + \mu < 2$$

where $I(\lambda, \mu)$ stands for the same infimum as in (75) but with the constraints $\int_{\mathbb{R}^3} u^2\, dx = \lambda$, $\int_{\mathbb{R}^3} v^2\, dx = \mu$. The proof of these strict inequalities uses the fact that if $\lambda = 0$ or if $\mu = 0$ then $I(\lambda, \mu) = 0$ while if $0 < \lambda < 1$, $0 < \mu < 1$ then $I(\lambda, \mu) = \lambda\mu E\left(\frac{1}{\lambda}, \frac{1}{\mu}\right)$ where

$$E(s, t) = \operatorname{Inf}\left\{ s \int_{\mathbb{R}^3} |\nabla u|^2\, dx + t \int_{\mathbb{R}^3} |\nabla u|^2\, dx + - \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} u^2(x)\, V(x - y)\, v^2(y)\, dx\, dy / u, v \in H^1(\mathbb{R}^3)\,, \int_{\mathbb{R}^3} u^2\, dx = \int_{\mathbb{R}^3} v^2\, dx = 1 \right\}$$

and thus $E(s, t)$ is nondecreasing with respect to s or to t. Observing next that $\lambda\mu + (1 - \lambda)(1 - \mu) < 1$ if $0 < \lambda < 1$, $0 < \mu < 1$ we deduce the above strict subadditivity inequality by remarking that

$$E(1, 1) \leqslant E\left(\frac{1}{\lambda}, \frac{1}{\mu}\right), \qquad E(1, 1) \leqslant E\left(\frac{1}{1 - \lambda}, \frac{1}{1 - \mu}\right).$$

We conclude this section by mentioning that the study of various nucleii seems to indicate that the mechanism we illustrated by the simple example 1 apparently does not cover all the possible ways the spherical symmetry is broken. To explain this claim, let us first explain how spin dependence (and spin-orbit forces) makes the above description a bit more complicated. Indeed, in such a case, the sequence of HF levels is typically of the following form (1s 1/2 multiplicity 2, 1p 3/2 multiplicity 4, 1p 1/2 multiplicity 2, 1d 5/2 multiplicity 6, 2s 1/2 multiplicity 2...) where the states (levels) are labelled as it is usual by the set n, l, j where j denotes the eigenvalue of the total angular momentum $\vec{j} = \vec{e} + \vec{s}$. Thus, the degeneracy (multiplicity) of the level (n, l, j) is $2j + 1$. With this scheme one checks that both nucleii ${}^{12}_{6}C$ and ${}^{28}_{14}S$ have nucleons numbers compatible with a spherical HF solution built on the lowest levels or eigenvalues. Yet, the HF computations lead to solutions which are not spherical but deformed. In fact they correspond to axially deformed shapes i.e. solutions with cylindrical symmetry $\left(\frac{x^2 + y^2}{a^2} + \frac{z^2}{c^2} = 1\right)$ which are prolate $\left(\text{i.e. } \frac{c}{a} > 1, \text{ oblate corresponding to } \frac{c}{a} < 1\right)$ — see M. Girod and B. Grammaticos [21]; K. Kumar, Ch. Lagrange, M. Girod and G. Grammaticos [35].

X. EXTERNAL FIELD METHOD

To present the external field method it is worth saying a few words on the numerical computation of HF minimization problems. Because of the quite complicated form of the functionals one has to minimize, some numerical methods which are currently used (typically Galerkin type methods based on spherical harmonics, or two basis of spherical harmonics centered at different points...) make difficult to avoid symmetries and seem to favor the possible local minima with spherical or cylindrical symmetry. And in all cases the numerical methods break the translation invariance. These remarks explain why the standard problem in the minimization of nonconvex functions of avoiding local minima in order to find the absolute minimum seems even more acute in HF problems. One idea to avoid this difficulty is to deform the shape of the density by an external field acting on the system as an additional constraint. As we will explain below this approach is not only useful for numerical purposes but is also relevant for physics.

To explain the principle of the external field method, we consider a C^1 functional on a manifold M, bounded from below and we are interested in the minimization problem

$$E = \operatorname{Inf}\{\mathscr{E}(u) \mid u \in M\}. \tag{76}$$

Now if Q is some given C^1 functional, and $q \in \mathbb{R}$ we consider the same minimization problem where we add the constraint $Q(u) = q$ (which in HF problems represents the action of the external field)

$$E(q) = \text{Inf}\{ \mathscr{E}(u)/u \in M,\ Q(u) = q \} \tag{77}$$

It is obvious that $E = \text{Inf}\ E(q)$ and that if this infimum is achieved at q_0 and if $E(q_0)$ is achieved at some u_0 then u_0 is a minimum of (76) But observe also that if we assume that at some q_0, E is differentiable, $E'(q_0) = 0$ and that for q near q_0 $E(q)$ is achieved at some u_q differentiable with respect to q at q_0, then u_{q_0} is a critical point of $\mathscr{E}$ Indeed, u_{q_0} being a minimum of $E(q_0)$, there exists a Lagrange multiplier θ such that

$$\mathscr{E}'(u_{q_0}) = \theta Q'(u_{q_0}) \tag{78}$$

while if we denote by $v_0 = \left.\dfrac{du_q}{dq}\right|_{q=q_0}$ then differentiating the relations $Q(u_q) = q$, $\mathscr{E}(u_q) = E(q)$ we obtain

$$1 = Q'(u_{q_0}).v_0\,, \qquad 0 = \mathscr{E}'(u_{q_0}).v_0$$

Therefore applying v_0 to the equality (78), we obtain $\theta = 0$ and we conclude

Finally, let us observe that if $E(q)$ admits a minimum at q_0, then roughly speaking u_{q_0} is a local minimum of $\mathscr{E}$ Hence, this method appears to be a way to explore the local minima of $\mathscr{E}$ Of course, one may use several constraints instead of one i e

$$Q_i(u) = q_i \quad \text{for} \quad 1 \leqslant i \leqslant k$$

In HF problems in Nuclear Physics, these forced constraints Q are mostly taken to be linear in ρ i e

$$Q(\varphi_1, \ \ , \varphi_A) = \int_{\mathbb{R}^3} Q(x)\, \rho(x)\, dx \tag{79}$$

for some function (field) Q on $\mathbb{R}^3$ In addition, they are chosen in such a way that the added constraint measures the deformation of the nucleus (we give an example below) Hence, if one computes

$$E(q_1, \ \ , q_k) = \text{Inf}\left\{ E(\varphi_1, \ \ , \varphi_A) \Big/ \int_{\mathbb{R}^3} \varphi_i\, \varphi_j^*\, dx = \delta_{ij}\,, \right.$$
$$\left. Q_l(\varphi_1, \ \ , \varphi_A) = q_l \quad \text{for} \quad 1 \leqslant l \leqslant k \right\} \tag{80}$$

for some HF functional E and where $Q_1, \ldots, Q_k$ are k external fields, then it is possible to describe the energy of nuclei (even heavy ones) as a function of its shape. And this seems to be relevant to the study of fission isomers and fission barriers (see J. F. Berger, M. Girod and D. Gogny [6], M. Girod and B. Grammaticos [21]).

We now conclude this section by a simple example of an external field. In (79) one can take for $Q(x)$

$$Q(x) = (x_1^2 + x_2^2 - 2\,x_3^2)\,\zeta(r) \tag{81}$$

where $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ and $\zeta(r)$ is some kind of cut-off function such that Q is bounded on $\mathbb{R}^3$. Of course, it is possible to analyze problems like (80) by the concentration-compactness method and to write down necessary and sufficient conditions involving strict sub-additivity conditions. But the verification of these conditions seems to be even more out of reach than for the HF problems we considered in the preceding sections.

XI. TIME-DEPENDENT HARTREE-FOCK EQUATIONS

The time-dependent Hartree-Fock equations (TDHF in short) are coupled nonlinear Schrödinger equations. Given any HF functional $E(\varphi_1, \ldots, \varphi_A)$ as in the preceding sections, TDHF equations may be written as follows

$$i\frac{\partial \varphi_k}{\partial t} + \frac{\partial E}{\partial \varphi_k}(\varphi_1, \ldots, \varphi_A) = 0 \quad \text{on} \quad \mathbb{R}^3 \times (0, \infty)\,, \quad 1 \leqslant k \leqslant A\,. \tag{82}$$

Of course, to solve (82) one has to add initial conditions

$$\varphi_k(x, 0) = \varphi_k^0(x) \quad \text{on} \quad \mathbb{R}^3\,, \quad 1 \leqslant k \leqslant A \tag{83}$$

where φ_k^0 is given ($1 \leqslant k \leqslant A$).

For example if E is given by (21), then (82) may be rewritten as

$$i\frac{\partial \varphi_k}{\partial t} - \frac{\hbar^2}{m}\Delta\varphi_k - \frac{\beta}{2}\operatorname{div}[\rho\,\nabla\varphi_k] + W\varphi_k = 0 \quad \text{on} \quad \mathbb{R}^3 \times (0, \infty)\,, \qquad 1 \leqslant k \leqslant A$$

where

$$W = -\,\alpha\rho + \frac{\beta}{2}\tau - \frac{\gamma}{4}\Delta\rho + \delta\rho^2\,.$$

Concerning the motivations in Nuclear Physics, for studying TDHF, we refer the reader to H. Flocard [16].

We will not give results concerning the resolution of the Cauchy problem (82), (83) : let us just mention the works by J. Ginibre and G. Velo [18], [19], [20]; for all interactions except Skyrme's there is no special difficulty to solve (82)-(83). Many mathematical results on systems like (82) are based on the various conservation laws satisfied by solutions of (82) : for example multiplying (82) respectively by φ_k^* and taking the imaginary part, and by $\frac{\partial \varphi_k}{\partial t}$ and taking the real part one finds integrating over $\mathbb{R}^3$

$$\int_{\mathbb{R}^3} |\varphi_k|^2 \, dx \quad \text{is independent of } t\,, \quad 1 \leqslant k \leqslant A \tag{84}$$

$$E(\varphi_1, \ldots, \varphi_A) \quad \text{is independent of } t\,. \tag{85}$$

Similarly, one obtains that $\int_{\mathbb{R}^3} \varphi_k \, \varphi_l^* \, dx$ is independent of t for $1 \leqslant k, l \leqslant A$.

We next observe that solutions of HF equations (up to unitary transform) lead to stationary solutions of TDHF equations where stationary means that ρ, τ are independent of t : more precisely we have seen in the preceding sections that we may write the HF equations as

$$\frac{\partial E}{\partial \varphi_k}(\varphi_1, \ldots, \varphi_A) = \varepsilon_k \, \varphi_k \text{ on } \mathbb{R}^3\,, \quad \text{for} \quad 1 \leqslant k \leqslant A\,.$$

Then obviously $\theta_k(x, t) = e^{i\varepsilon_k t} \, \varphi_k(x)$ $(1 \leqslant k \leqslant A)$ defines a solution of (82).

In particular, any minimum of the HF minimization problems leads to a stationary solution of TDHF equations. It is shown in T. Cazenave and P. L. Lions [12] that, if the subadditivity conditions given in the preceding sections via the concentration-compactness arguments hold, minima of HF minimization problems are orbitally stable in TDHF equations. Let us also point out that similar arguments show that minima of the HF minimization problems with additional symmetry constraints (see section VIII) are orbitally stable with respect to perturbations with the same symmetries.

But since all solutions of HF equations lead to stationary solutions of TDHF equations, the study of all possible solutions of HF equations presents some interest. In particular one may look for critical points of $E(\varphi_1, \ldots, \varphi_A)$ with the additional orthogonality constraints. The only approach we know one might try is through min-max principles as it is done in H. Berestycki and P. L. Lions [5], P. L. Lions [38], [39], [32] for related problems. This approach requires spherical symmetry of the functions $(\varphi_1, \ldots, \varphi_A)$. We only have very partial existence results in that direction.

In fact Nuclear Physics considerations indicate that it would be interesting to find all periodic solutions of TDHF : again one has to define the precise meaning of periodic solutions. For example, if no differences are made between neutrons and protons, a solution of (82) is said to be periodic of period T if there exists a unitary transform U such that

$$(\varphi_1(T), \ldots, \varphi_A(T)) = U(\varphi_1(0), \ldots, \varphi_A(0)) \text{ on } \mathbb{R}^3 .$$

Observe that this implies that the densities ρ, τ are indeed periodic of period T (in the usual sense). In fact, an even more general (possibly) notion of periodic solutions consists in requiring the density $\rho(x, y)$ to be periodic. It seems, at least numerically, that there are many periodic solutions of TDHF equations and this is another major open question.

A final remark on this topic concerns the possibility of having stationary solutions of TDHF equations which are not obtained through solutions of HF equations. We illustrate this possibility on a simple example of a system of two nonlinear equations.

Example : We consider the following system of two coupled nonlinear Schrödinger equations

$$\begin{cases} i\varphi_t - \Delta\varphi = \rho^{\gamma-1}\varphi & \text{on } \mathbb{R}^3 \times (0, \infty) \\ i\psi_t - \Delta\psi = \rho^{\gamma-1}\psi & \text{on } \mathbb{R}^3 \times (0, \infty) \end{cases} \tag{86}$$

where $\rho = (|\varphi|^2 + |\psi|^2)$ and $1 < \gamma < 5/3$.

Let $\omega, m > 0$; we look for solutions of (86) of the form

$$\varphi(x, t) = e^{-i\omega t}(\cos mtu(x) + \sin mtv(x))$$
$$\psi(x, t) = e^{-i\omega t}(-\sin mtu(x) + \cos mtv(x)) .$$

And we find the following nonlinear system for u, v

$$\begin{cases} -\Delta u + imv + \omega u = \rho^{\gamma-1} u \text{ in } \mathbb{R}^3 \\ -\Delta v - imu + \omega v = \rho^{\gamma-1} v \text{ in } \mathbb{R}^3 . \end{cases} \tag{87}$$

Observe that if we show there exist solutions (u, v) of (87) then the above $\varphi(x, t)$, $\psi(x, t)$ yield stationary solutions of (86) (ρ is independent of t). However, if φ, ψ were solutions of (86) built through the stationary analogue of HF equations, this would imply that $v = -iu$. Thus, we want to exhibit solutions of (87) with $v \not\equiv -iu$. To this end we consider the following minimization problem

$$I = \operatorname{Min}\left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + |\nabla v|^2 + \omega |u|^2 + \omega |v|^2 + \operatorname{Re}(imv\bar{u})\, dx / u, v \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} \rho^\gamma\, dx = 1 \right\}. \quad (88)$$

This problem is solved as in [33] by the concentration-compactness arguments and thus there exists a minimum (u, v) of (88). Now, if we have $v \equiv -iu$, this would imply

$$I \geqslant \operatorname{Min}\left\{ \int_{\mathbb{R}^3} 2|\nabla u|^2 + 2\omega |u|^2 + m|u|^2\, dx / u \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |u|^{2\gamma}\, dx = 2^{-\gamma} \right\}$$

and this last minimum is strictly larger than

$$2 \operatorname{Min}\left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + \omega |u|^2\, dx / u \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |u|^{2\gamma}\, dx = 2^{-\gamma} \right\} =$$

$$= \operatorname{Min}\left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + \omega |u|^2\, dx / u \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |u|^{2\gamma}\, dx = 1 \right\}$$

On the other hand, we have taking $v = 0$ in (88)

$$I \leqslant \operatorname{Min}\left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + \omega |u|^2\, dx / u \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |u|^{2\gamma}\, dx = 1 \right\}$$

and the contradiction proves our claim on the existence of a solution of (87) with $v \not\equiv -iu$.

XII. HARTREE-FOCK-BOGOLYUBOV APPROXIMATION

In this section, we want to present a different approach to the study of nucleii namely the so-called Hartree-Fock-Bogolyubov approximation (N. N. Bogolyubov [10], C. Bloch and A. Messiah [9], J. B. Bardeen, L. N. Cooper, and J. R. Schrieffer [3]). We will not attempt here to explain the Hartree-Fock-Bogolyubov method and we refer to the interested reader to J. Dechargé and D. Gogny [14], J. G. Valatin [47]. We will only describe the typical minimization problem arising in this theory which may be thought of as an improved approximation of the A-body problem considered in section II. To simplify, we will again ignore the spin dependence and spin-orbit forces. The minimizing set is given by

$$M = \left\{ (u_i, v_i)_{i \geq 1} \in L^2(\mathbb{R}^3) \times H^1(\mathbb{R}^3) \, ; \int_{\mathbb{R}^3} u_i \, v_j^* + u_j^* \, v_i \, dx = 0 \right.$$
$$\left. \int_{\mathbb{R}^3} u_i \, u_j^* + v_i \, v_j^* \, dx = \delta_{ij} \text{ for all } i, j \geq 1 \, ; \sum_{i \geq 1} \int_{\mathbb{R}^3} | v_i |^2 \, dx = A \right\} .$$

We now introduce the Hartree-Fock-Bogolyubov problem (HFB in short)

$$\operatorname{Inf} \left\{ \int_{\mathbb{R}^3} \frac{\hbar^2}{2m} \sum_{i \geq 1} | \nabla v_i |^2 \, dx + \frac{1}{2} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} \rho(x) \, V(x-y) \, \rho(y) \, dx \, dy + \right.$$
$$- \frac{1}{2} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V(x-y) \, | \rho(x,y) |^2 \, dx + \frac{1}{2} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V(x-y) \, | \kappa(x,y) |^2 \, dx \, dy /$$
$$\left. (u_i, v_i)_{i \geq 1} \in M \right\}$$

where

$$\rho(x) = \sum_{i \geq 1} | v_i(x) |^2 \, , \quad \rho(x, y) = \sum_{i \geq 1} v_i(x) \, v_i^*(y) \, ,$$

$\kappa(x, y) = \sum_{i \geq 1} u_i(x) \, v_i^*(y)$ for $x, y \in \mathbb{R}^3$. And one may choose for example (as in [14]) the potential

$$V(x) = \sum_{i = 1,2} W_i \exp(- | x |^2 / \mu_i^2)$$

where W_i, μ_i are constants.

Most of the results, remarks and open problems given in the preceding sections may be adapted to the study of problem (89).

Before explaining how we may apply the concentration-compactness program on this problem, let us first mention the important connection between the above problem and more standard HF problems. Deriving the Euler-Lagrange equations of the above minimization problem (which by the way are called Hartree-Fock-Bogolyubov equations) one sees immediately that if $(\overline{v}_1, \ldots, \overline{v}_A)$ is a solution of the HF equations then choosing $v_i \equiv \overline{v}_i$ for $1 \leq i \leq A$,

$v_i \equiv 0$ for $i > A$, $u_i \equiv 0$ for $1 \leqslant i \leqslant A$, u_i arbitrary satisfying

$$\int_{\mathbb{R}^3} u_i u_j^* \, dx = \delta_{ij}$$

for $1 + A \leqslant i, j$, we find a particular (" trivial ") solution $(u_i, v_i)_{1 \leqslant i}$ of the HFB equations. In some vague sense, the HFB problem contains the HF problem.

We now conclude with a brief explanation on the way we may apply the concentration-compactness arguments to the above problem. We apply the usual concentration-compactness lemma to the density ρ. And we see that minimizing sequences $(u_i, v_i)_{i \geqslant 1}$ of the above minimization problem are compact up to a translation in $L^2(\mathbb{R}^3) \times H^1(\mathbb{R}^3)$ if and only if

$$I < I(M_1, M_2, N) + I(M_1', M_2', -N)$$

for all hermitian matrices M_1, M_2, M_1', M_2', N satisfying $M_1, M_2, M_1', M_2' \geqslant 0$,

$$\mathrm{Tr}(M_1) \in [0, A], \quad \mathrm{Tr}(M_1') = A - \mathrm{Tr}(M_1), \quad M_1 + M_2 + M_1' + M_2' = \mathbb{1}$$

and

$$|(N\xi, \xi)| \leqslant (M_1 \xi, \xi)^{1/2} (M_2 \xi, \xi)^{1/2}, \quad \forall \xi \in l^2,$$

where in addition $0 \neq M_1 + M_2$, $M_1 + M_2 \neq \mathbb{1}$. In the above inequality

$$I = \mathrm{Inf}\{ I(M_1, M_2, 0)/M_1, M_2 \geqslant 0, \; M_1 = M_1^*, \; M_2 = M_2^*, \; M_1 + M_2 = \mathbb{1}, \; \mathrm{Tr}(M_1) = A \}$$

and finally, denoting by $P(i,j)$ the i, j component of the matrix $P(1 \leqslant i, j)$, the definition of $I(M_1, M_2, N)$ is given by

$$I(M_1, M_2, N) = \mathrm{Inf}\Big\{ \int_{\mathbb{R}^3} \sum_i \frac{\hbar^2}{2m} |\nabla v_i|^2 \, dx + \frac{1}{2} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} \rho(x) V(x - y) \rho(y) \, dx \, dy - \frac{1}{2} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V(x - y) \times |\rho(x, y)|^2 \, dx \, dy + \frac{1}{2} \int_{\mathbb{R}^3 \times} \int_{\mathbb{R}^3} V(x - y) |\kappa(x, y)|^2 \, dx \, dy / (u_i, v_i) \in L^2 \times H^1,$$

$$\int_{\mathbb{R}^3} v_i v_j^* \, dx = M_1(i,j) , \quad \int_{\mathbb{R}^3} u_i u_j^* \, dx = M_2(i,j) ,$$

$$\left. \int_{\mathbb{R}^3} u_i v_j^* + u_j v_i^* \, dx = N(i,j) \right\}$$

In fact, as in the case of HF problems, using the various invariances of the above problems it is possible to restrict the above strict subadditivity inequalities to a particular class but we will not pursue this matter here

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