# **Review of mean-field theory**

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## ABSTRACT

During the last thirty years, the Joliot-Curie school (EJC) has significantly contributed to the diffusion of knowledge originally at the French-Belgium level and more recently to a wider international audience. Certainly due to the important historical contribution of the francophone community to the mean-field approach (Vautherin and Brink, Phys. Rev. C5 (1972), Decharge and Gogny, Phys. Rev. C21 (1980)), mean-field theory are among the most popular topics in this school. The goal of the present one hour lecture was to provide an overview of this approach applied to low energy nuclear physics. In the 2011 school, I have tried to focus on the key concepts disregarding sometimes important conceptual and technical details. For those who are interested in them, I strongly recommend to consult the EJC website (http://www.cenbg.in2p3.fr/joliot-curie/) where numerous excellent lectures (originally in french and more recently in english) can be found (see conclusion).

Here, I first introduce reasons why the nuclear many-body problem is one of the most complex problem in many-body physics. Despite this complexity, many experimental observations points out that nucleons can, in a good approximation, be regarded as a system of independent particles moving in a self-consistent mean-field. Unfortunately, the usual theory, i.e. the Hartree-Fock theory, that is the natural way to replace a many-body problem into a one-body problem miserably fails in nuclear physics. To overcome this difficulty, nuclear physicists make use of Density Functional Theory, generally called Energy Density Functional (EDF). Basic aspects of the EDF are introduced here for beginners. To make the EDF approach systematic and predictive in a rather simple and numerically economic way, this approach use and abuse of symmetry breaking. Symmetry breaking is an elegant technique to incorporate important correlations like pairing that would be difficult to include otherwise. Finally, the necessity to ultimately restore broken symmetries within EDF using configuration mixing is discussed. In this review, I will mainly concentrate on nuclear structure aspects. However, the EDF is not restricted to ground state properties but is expected to provide a unified microscopic framework able to address the diversity of phenomena taking place in nuclei from nuclear structure to nuclear reactions or nuclear astrophysics: nuclear spectroscopy, small and large amplitude dynamics, equilibrium and non-equilibrium thermodynamics.

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## I. INTRODUCTION: COMPLEXITY AND SIMPLICITY OF THE NUCLEAR MANY-BODY PROBLEM

Nuclei are composite mesoscopic objects formed of neutrons and protons that are themselves composed of quarks (see left side of figure 1). Fortunately, the energy scale associated to quark degrees of freedom is well separated from the energy scale associated to nucleonic degrees of freedoms and for low energy nuclear physicists, nucleons can be regarded as elementary particles interacting through the strong nuclear force. Nucleons are quantum fermionic objects, their wave-function can be decomposed into a space (or momentum), a spin  $\sigma = \uparrow, \downarrow$  and isospin  $\tau = n, p$ , i.e.  $\phi_{\text{nucleon}} \equiv \phi(\mathbf{r}, \sigma, \tau)$ . The nuclear many-body problem is particularly complex due mainly to the following reasons:

• The nuclear interaction itself is very specific. In figure 1 (right), the two-body wavefunction is shown as a function of the relative distance between nucleons. Different curves corresponds to the different total spin S and isospin T of the two-nucleon



FIG. 1: Left: Schematic illustration of the hierarchic composition of nuclei into nucleon and nucleon into quarks. Right: Evolution of the nuclear two-body interaction as a function of the relative distance between nucleons. The different curves corresponds to different total spin and isospin channels.

wave-function. As illustrated by this figure, the nuclear force strongly depends on the spin-isospin channels, with in particular a strong tensor components. One of the difficulties is the existence of a strong repulsion at short distance, the so-called hard-core. This repulsion is actually exponentially divergent and requires specific treatments before using it in a many-body theory (like Brueckner-Hartree-Fock (Fetter and Walecka book (1991)) and more recently renormalization techniques (Bogner et al, Phys. Rep. (2003), Epelbaum et al, Rev. Mod. Phys. (2009)). Besides the nuclear interaction, protons, being charged particles, interact through the Coulomb force. Note in addition that recently, the possible role of a three-body forces, whose property is largely unknown, has been pointed out (Nogga et al, Phys. Rev. Lett. (2000)).

• Most nuclei are mesoscopic systems, which means that there are neither few- nor infinite-body systems. The antisymmetric wave-function associated to nuclei can be written as (for simplicity spin and isospin components are omitted):

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_{12}, \mathbf{r}_{13}, \cdots, \mathbf{r}_{123}, \cdots)$$
(1)

where  $\mathbf{r}_i$  denotes the position of the nucleon "i",  $\mathbf{r}_{ij}$  denotes the relative distance between nucleon "i" and "j", ... For a system of N particles, the size  $\Omega$  of the wavefunction components exploded and is schematically given by  $\Omega = N! \times [\text{size of the} nucleon Hilbert space]$ . Even if impressive progress have been made in the last decades along this line, the explosion of degrees of freedoms to be treated plagued exact solution of the nuclear many-body problem through ab-initio techniques to a restricted area of the nuclear chart. in addition, nucleons are not enough to take advantages of possible techniques and simplifications used in infinite systems. Finite size effects are important in nuclei leading to highly interesting and non-trivial effects.

In the following, the Energy Density Functional theory is introduced where the initial interacting many-body problem is replaced by an independent particle (resp. quasiparticle) problem and where the important quantity is the one-body normal (resp. normal and anomalous) density  $\rho(r, r')$  that contains the information on one-body observables.

#### A. Simple aspects of complex nuclei

Surprisingly enough in view of the complexity of the interaction, many observations in nuclei can be understood assuming that the nucleons behave as independent particles in an effective one-body potential. Several aspects of the independent particle manifestation in nuclei are illustrated here.

#### 1. One-body density in nuclei with electron scattering experiments

When an electron is send onto a nucleus, it feels the long-range Coulomb force induced by the protons. As a consequence, electrons are ideal probes to determine the charge density (proton density) of nuclei. At suitable beam energies, electron beams have been used to determine the charge density profile  $\rho_p(r)$  of various nuclei. Experimentally, a high resolution spectrometer is used to determine the net momentum transfer q while the electron passes by the nucleus. The density distribution (bottom part), shown in Figure 2, are obtained from cross-section analyses of the (e,e') experiments. It corresponds approximately to the inverse Fourier transform of the momentum distribution deduced from the cross section F(q) shown in the top part of the Figure 2. The F(q) pattern looks similar to Airy function obtained in optics by the diffusion from a semi-transparent object. Large q values give access to the central part of the density, while small q gives information on the surface of the nucleus. Examples of density profiles obtained from light to heavy nuclei are shown in the same figure (bottom left). From this figure, we see that the density inside the nucleus is almost constant and equal to 0.16 fm<sup>-3</sup>.

Density profiles along the nuclear chart can be accurately parameterized with a Fermi shape:

$$\rho(r) = \frac{\rho_0}{1 + \exp(\frac{r - R_0}{a})}$$
(2)

where  $R_0$  is the radius at half density while *a* is the diffuseness of the surface. Typical estimates give  $R_0 = 1.2A^{1/3}$  fm and a = 0.5/0.6 fm.

Within a microscopic approach based on the independent particle picture, the densities presented in figure 2 are nothing but the local part of the one body density matrix, i.e.  $\rho(r) \equiv \rho(r, r')|_{r=r'}$  (see discussion below).

#### 2. Shell effects

One of the most evident fingerprint of the importance of single-particle effects in nuclei is the existence of shell effect. As the electron beam energy increases (typically 500MeV) thinner details of the structure of the atomic nucleus can be probed, such as the nucleons themselves. High energy electrons can be used to knock-out individual protons located on



FIG. 2: (Color online) Top: illustration of electron scattering experiments. After interacting with the nucleus, the electron is scattered with a momentum different from the initial one. From the properties of the electron (form factor), the density of proton in the nucleus can be deduced (bottom-left). In this figure, the proton density is multiplied by the factor A/Z to get the total density (adapted from Sorlin, EJC (2009)). We see that the density at the center of the nucleus is almost constant and equal to 0.16 fm<sup>-3</sup>. In the bottom left, the equation of state of the infinite nuclear matter is also shown. The equilibrium properties can be seen as an extrapolation of the observation made in nuclei as the mass A and volume V go to infinity while keeping their ratio constant.

the various shells inside the nucleus, i.e. an electron induces the ejection of a proton. This is the (e,e',p) technique illustrated in Figure 3 with a lead target. The energy of the ejected proton present peaks at well defined position signing the fact that it was initially located on well defined quantum orbitals. Different peaks, labelled as  $1/2^+$ ,  $3/2^+$ ,  $11/2^+$  and  $5/2^+$ , are shown in Figure 3. They correspond to knocked-out protons from the  $s^{1/2}$ ,  $d^{3/2}$ ,  $h^{11/2}$ , and  $d^{5/2}$  orbits. The amplitude of the each peak scales roughly with the expected degeneracy of the orbits, i.e. 2j + 1. For instance, the signal from the  $h^{11/2}$  orbit (which should contain 12 protons) is the largest, while the  $s^{1/2}$  which can contain only two protons is about 5 times smaller.

The (e,e',p) experiments shows that nucleons behaves very much like independent particle occupying orbits of a single-particle potential. Their wave-function can then be obtained by solving an single-particle Schrödinger equation of the form:

$$\left\{\frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) + f(\mathbf{r})\vec{l}.\vec{s}\right\} |\varphi_{\alpha}\rangle = \varepsilon_{\alpha}|\varphi_{\alpha}\rangle \tag{3}$$

The potential  $V(\hat{\mathbf{r}})$  can be accurately considered as a spherical symmetric Wood-Saxon



FIG. 3: (Color online) Right: Sequence of proton orbits in the (Z=82)  $^{208}$ Pb nucleus derived from the proton knock-out induced by electrons. Irregular spacing between shells is evidenced. The number of protons  $N_p$  per peak scales roughly with the occupancy of the states. Left: Illustration of the level scheme assuming that the one-body potential identifies with a Harmonic Oscillator (H.O.) for the one-body potential. The degeneracy is removed due to the presence of the l(l + 1)term and  $\vec{l}.\vec{s}$  spin orbit term (adapted from Sorlin, EJC (2009)).

potential given by:

$$V(r) = \frac{V_0}{1 + \exp(\frac{r - R_0}{a})}$$
(4)

where  $V_0 \simeq -50$  MeV. The term  $f(\mathbf{r})\vec{l}.\vec{s}$  is known as the spin-orbit coupling term. As illustrated in figure 3 for the harmonic oscillator case, we do expect that shell gaps exist at specific particle number 8, 20, 40... due to the spin-orbit term shell gaps are modified and are observed at 8, 20, 28, 50, 82,... this numbers being called magic numbers. A further illustration of the appearance of magic numbers is given in fig. 4, where the separation energy (i.e. the difference between the energy of the nucleus and the energy of a nucleus with one nucleon removed) is displayed along the nuclear chart.

## B. Why is the independent particle valid in complex nuclei?

At first glance, it is surprising that nuclei might be considered as independent particles interacting through an effective mean-field potential. Indeed, nucleons interact through the so-called strong interaction presenting a strong repulsive short range component. A first hint of why it is possible is given above: the interaction that two nucleons feels inside the nucleus differs significantly from the one they feel when they are outside the nucleus. This



FIG. 4: Top: One neutron Separation energy  $S_n$  in nuclei as a function of neutron number for even-even nuclei. The lines correspond to nuclei for same proton number. Bottom: The lines display the difference between separation energy for the same sets of neighboring even-even nuclei. The horizontal dashed lines correspond to magic numbers 8, 20, 28, 50, 82 and 126.

could be summarized as the interaction is strongly renormalized by the medium effects.

#### 1. Interaction between particle and phase-shift

The best way to characterize the interaction between two particles is to make them collide and detect the product of the reaction (see illustration in Fig 5 (left)). In scattering theory, the cross section is best studied by introducing the eigenstates of the two-body problem, denoted by  $\Psi_{\text{scat}}$ . Since detectors are positioned at almost infinite distance, the probability to detect a particle at a given position is only sensitive to the asymptotic behavior of the wave-function, i.e. (see for instance Lacroix, EJC (2009))

$$\Psi_{\rm scat}(\mathbf{r}) \xrightarrow{\mathbf{r} \to \infty} e^{ikz} + f(\theta, \varphi) \frac{e^{ikr}}{r}$$

where we recognize the superposition of the incident wave-function of a particle with an energy  $E = \frac{\hbar k^2}{2\mu}$  and a scattering wave. Then, the cross section detected at given angles  $\theta$  and  $\varphi$  (where these angles correspond to spherical coordinates, z being the beam axis), is related to the scattering amplitude through the simple relation  $\sigma_k(\theta, \varphi) = |f(\theta, \varphi)|^2$ . Taking advantage of the fact that the nuclear interaction depends only on the relative distance

between nucleons, the scattering wave-packet can be further decomposed on eigenstates with good angular momentum as

$$\Psi_{\text{scat}}(\mathbf{r}) = \sum_{nlm} c_{nlm} \frac{u_{nl}(r)}{r} Y_{lm}(\theta, \varphi).$$

We are then left with the study of the asymptotic behavior of the  $u_{nl}(r)$  that is usually written as

$$u_{nl}(r) \stackrel{\mathbf{r} \to \infty}{\sim} \sin\left(kr - l\frac{\pi}{2} + \delta_l(k)\right)$$

where  $\delta_l(k)$  denotes the phase-shift at a given l and energy (note that here for the sake of simplicity, spinless particles have been considered). The physical meaning of the phase-shift is illustrated in figure 5 (Top-Right). As a final result, the cross-section integrated over the angles can be simply written as

$$\sigma(k) = \frac{4\pi}{k^2} \sum_{l} (2l+1) \sin^2[\delta_l(k)].$$

#### 2. Free versus in-medium scattering

Let us now imagine two types of experiments. In one case, one nucleon collide with another nucleon that are completely isolated from the rest of the world (top-left of figure 5). In the other case, the target nucleons is immerged inside a nucleus (bottom-left of figure 5). When two nucleons are surrounded by other nucleons, the associated wave function (red dashed curve) looks very much like an independent particle case (black solid curve). This stems from a combined effects of the Pauli principle that blocks accessible configurations for the two nucleons and the properties of the force itself. This simple analysis can be used for instance to reconcile on one hand the strength of the interaction and the independent particle picture validity in nuclei. In this figure (Bottom-right), the nucleon mean-free path  $\lambda$  of a nucleon inside a nucleus is also shown. This distance could be regarded as the distance a nucleon travels without encountering collisions. The bigger  $\lambda$  is, the more independent could be regarded the particles.  $\lambda$  is given by  $\lambda = 1/(\sigma \rho_0)$  where  $\sigma$  is the cross section. We see in figure 5 that  $\lambda$  is much higher in the medium than in the case of free nucleon again showing that the surrounding nucleons are screening direct collisions.

## II. FROM MANY-BODY TO INDEPENDENT PARTICLE PICTURE : THE HARTREE-FOCK METHOD

Let us start from a very general Hamiltonian describing N interacting particles

$$H = \sum_{i} T(i) + \sum_{i < j} V^{(2)}(i, j) + \sum_{i < j < k} V^{(3)}(i, j, k)$$
(5)

where the first term is corresponds to the sum of the kinetic energies of the particles, the second term denotes the two-body interaction, the third term is the three-body interaction...

The quantum description of such a system requires a priori the knowledge of its N-Body wave function  $\Psi^*({\mathbf{r}_i}, t)$  or more generally its N-body density matrix denoted by  $D({\mathbf{r}_i}, t)$ .  ${\mathbf{r}_i}$  is a short-hand notation for the particles coordinates  $(\mathbf{r}_1, \dots, \mathbf{r}_N)$ . The complexity of the Many-body problem comes from the number of degrees of freedom to consider. As



FIG. 5: (Color online) Left: Schematic illustration of the diffusion of one nucleon onto another nucleon with incident energy  $E = \frac{\hbar k^2}{2\mu}$ . Here,  $\mu$  is the reduced mass of the collision. In the top-left case, the target nucleon is isolated (free scattering case) while in the bottom-left case the collision happens inside a nucleus. Top-Right: Illustration of the effect of the interacting potential. Here a schematic two-body potential is used with a very sharp hard-core. The black solid curve is the reference two-body wave-function without any interaction at all. The blue solid curve is the free scattering nucleon case, i.e. without the surrounding nucleus, while the red dashed curve corresponds to the eigenstate with two-body interaction inside the nucleus. The phase-shift  $\delta_l(k)$  is directly related to the difference between the asymptotic behavior of the two curves. Bottom-right: nucleon mean-free path as a function of the energy of the nucleon. In a nucleus, due to the surrounding nucleons and more specifically the Pauli principle (in medium effect), the nucleon mean-free path is much larger than it would be in the absence of other nucleons.

mentioned earlier, except for very small number of particles, the total number of degrees of freedom to treat becomes prohibitory to get the exact ground state or the evolution of such a complex system. Therefore, we are forced to seek simplifications where much less relevant degrees of freedom are considered. the simplest approximation of a N-body problem is to assume that the particles do not interact with each others except through an average self-consistent mean-field. For fermionic systems, this is the so-called *Hartree-Fock* approximation. The philosophy of the independent particle approximation is depicted in Fig. 6.

In this approximation:

• The complex wave-function is replaced by a Slater determinant.



FIG. 6: Illustration of the independent particle approximation. The initial problem where particles interact two-by-two, three-by-three... is replaced by a simpler problem of single-particles interacting only through a self-consistent mean-field.

- Static and dynamical properties of the systems are obtained by solving N coupled equation on single-particle states.
- Slater determinants correspond to a specific example of trial states that are particularly suited to describe one-body observables.

## A. Many-Body wave-function, densities and relevant observables.

Here, we will consider operators using the second quantization. People that are not used to these mathematical tools can refer to textbook (see for instance (Blaizot and Ripka book (1986))). In second quantization, one-body, two-body, three-body... operators can be written as:

$$O^{(1)} = \sum_{ij} \langle i|O_1|j\rangle a_j^{\dagger} a_i$$
  

$$O^{(2)} = \frac{1}{4} \sum_{ij,kl} \langle ij|\tilde{O}_{12}|kl\rangle a_i^{\dagger} a_j^{\dagger} a_l a_k$$
  

$$O^{(3)} = \frac{1}{6} \sum_{ijk,lmn} \langle ijk|\tilde{O}_{123}|lmn\rangle a_i^{\dagger} a_j^{\dagger} a_k^{\dagger} a_l a_m a_m$$

Given a many-body state, all the information on one-body degrees of freedom are contained in the expectation values of the set of operators  $\{\langle a_i^{\dagger}a_j\rangle\}$ , the information on two-body degrees of freedoms are contained in the  $\{\langle a_i^{\dagger}a_j^{\dagger}a_la_k\rangle\}$ ... Let us assume for simplicity a single-particle basis of size  $\Omega$ . The type of degrees of freedom, associated sets of operators and their number are listed below:

Type	Quantities	Size	
One – body	$\{\langle a_i^{\dagger}a_j\rangle\}$	$[\Omega]^2$	
Two – body	$\{\langle a_i^\dagger a_j^\dagger a_l a_k  angle\}$	$[\Omega(\Omega-1)/2]^2$	(6)
Three – body	$\{\langle a_i^{\dagger}a_j^{\dagger}a_k^{\dagger}a_la_ma_n\rangle\}$	$[\Omega(\Omega-1)(\Omega-2)/3!]^2$	
		•••	

These components are of increasing complexity and corresponds to increasing order density matrices. The one-, two-, ... body density matrix (denoted hereafter by  $\rho^{(1)}$ ,  $\rho^{(2)}$ , ...) elements are defined through<sup>1</sup>:

$$\langle i|\rho^{(1)}|j\rangle = \langle a_j^{\dagger}a_i\rangle = \operatorname{Tr}(a_j^{\dagger}a_iD)$$

$$\langle kl|\rho^{(2)}|ij\rangle = \langle a_i^{\dagger}a_j^{\dagger}a_la_k\rangle = Tr(a_i^{\dagger}a_j^{\dagger}a_la_kD)$$

$$(8)$$

where D denotes the N-body density, that is given by  $D = |\Psi\rangle\langle\Psi|$ . With these definition, we see that expectation values of one, two-,... body observable can directly be expressed as:

$$\langle O^{(1)} \rangle = \operatorname{Tr}(O^{(1)}\rho^{(1)}) \langle O^{(2)} \rangle = \frac{1}{4} \operatorname{Tr}(\tilde{O}^{(2)}\rho^{(2)}) \dots$$

From this list, it can be seen that the number of degrees of freedom to treat becomes very large as more and more complex correlations are focused on. As a consequence, a manybody problem can rarely be treated exactly. Then, approximations where much less selected degrees of freedoms are selected are necessary.

#### B. Density matrices of a Slater determinant and reduction of the information

When the state of the system is described by a Slater determinant, then all the information on it is contained in the one-body density matrix  $\rho^{(1)}$  or in other words, any k-body density can be written as a function of the one-body density. Let us consider a Slater determinant written as:

$$|\Phi\rangle = \prod_{\alpha=1}^{N} c_{\alpha}^{\dagger} |-\rangle \tag{9}$$

<sup>&</sup>lt;sup>1</sup> be careful with the order.



FIG. 7: Schematic illustration of the reduction of of information to one-body degrees of freedom. Here, a system is suppose to evolve in time. When a Slater determinant is used instead of a more complex man-body state, this correspond to find an optimum path in the one-body space. It is worth mentioning that even the projected dynamics of the exact path will deviate from the mean-field approximation due to the accumulation of correlation beyond the independent particle picture.

associated to N orthogonal single-particle state  $|\varphi_{\alpha}\rangle$ . Then, we have the simple relationship between the matrix elements of the densities of order 2 and higher and the one-body density matrix elements <sup>2</sup>:

$$\rho_{ij;kl}^{(2)} = \rho_{ik}^{(1)} \rho_{jl}^{(1)} - \rho_{il}^{(1)} \rho_{jk}^{(1)} \tag{10}$$

$$\rho_{ijm;kln}^{(3)} = \rho_{ik}^{(1)} \rho_{jl}^{(1)} \rho_{mn}^{(1)} - \rho_{ik}^{(1)} \rho_{jn}^{(1)} \rho_{ml}^{(1)} - \rho_{in}^{(1)} \rho_{jl}^{(1)} \rho_{mk}^{(1)}$$

$$- \rho_{il}^{(1)} \rho_{jk}^{(1)} \rho_{mn}^{(1)} + \rho_{in}^{(1)} \rho_{jk}^{(1)} \rho_{ml}^{(1)} + \rho_{il}^{(1)} \rho_{jn}^{(1)} \rho_{mk}^{(1)}$$

$$\dots \tag{11}$$

Therefore, when the many-body wave-function is replaced by a Slater determinant, the twoand higher-body density matrix can be expressed as a function of the one-body density matrix elements, or said differently, they become a functional of the one-body density.

$$\rho_{12}^{(2)} = \rho_1^{(1)} \rho_2^{(1)} (1 - P_{12}) 
\rho_{123}^{(3)} = \rho_1^{(1)} \rho_2^{(1)} \rho_3^{(1)} (1 - P_{23} - P_{13}) (1 - P_{12}) \cdots$$

where here, the indices refers to the particle on which the matrix is applied, for instance:

$$\begin{split} \langle kl | \rho_1^{(1)} \rho_2^{(1)} | ij \rangle &= \langle k| \rho^{(1)} | i \rangle \langle l| \rho^{(1)} | j \rangle, \\ \langle kl | \rho_1^{(1)} \rho_2^{(1)} P_{12} | ij \rangle &= \langle kl | \rho_1^{(1)} \rho_2^{(1)} | ji \rangle = \langle k| \rho^{(1)} | j \rangle \langle l| \rho^{(1)} | i \rangle, \end{split}$$

 $<sup>^{2}</sup>$  Matrix elements can eventually be written in a more compact form using:

One says in that case that the information on the system is contained entirely in onebody degrees of freedom (DOF) and the knowledge of the system is reduced solely to the knowledge of  $\rho^{(1)}$ . In the following, when no ambiguity exists, we will simply use the notation  $\rho^{(1)} = \rho$ . This reduction of information can be seen as a projection onto the space of relevant degrees of freedom (see illustration 7), here the component  $\langle a_i^{\dagger} a_j \rangle$  while others (irrelevant DOF), like correlation beyond the independent particle picture are approximated.

Note finally that, in the case of Slater determinant wave-packet (Eq. 9), the one-body density can also be expressed in terms of the single-particle states as:

$$\rho_{ij} = \sum_{\alpha} \varphi_{\alpha}(i) \varphi_{\alpha}^{*}(j) \tag{12}$$

that can be formally written as  $\rho = \sum_{\alpha} |\varphi_{\alpha}\rangle \langle \varphi_{\alpha}|$ .

## C. Hartree-Fock theory

Since all density matrices express in terms of  $\rho$ , this is also the case for the energy. Here for the sake of simplicity, we consider only two-body Hamiltonian written as:

$$H = \sum_{ij} \langle i|T|j\rangle a_i^{\dagger} a_j + \frac{1}{4} \sum_{ij,kl} \langle ij|\tilde{v}|kl\rangle a_i^{\dagger} a_j^{\dagger} a_l a_k$$
(13)

where the two-body density matrix elements are anti-symmetrized. Using the different results given previously, the expectation value of H using a Slater determinant  $|\Phi\rangle$  becomes a functional of the one-body density matrix components <sup>3</sup>:

$$E_{\rm HF}[\rho] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \sum_{ij} t_{ij} \rho_{ji} + \frac{1}{4} \sum_{ij,kl} \tilde{v}_{ij,kl} (\rho_{ki} \rho_{lj} - \rho_{kj} \rho_{li})$$
  
$$= \sum_{ij} t_{ij} \rho_{ji} + \frac{1}{2} \sum_{ij,kl} \tilde{v}_{ij,kl} \rho_{ki} \rho_{lj}$$
  
$$= \operatorname{Tr}(t_1 \rho_1) + \frac{1}{2} \operatorname{Tr}(\tilde{v}_{12} \rho_1 \rho_2).$$
(14)

That can eventually be written in terms of single-particle states as

$$E_{\rm HF}[\rho] = E_{\rm HF}[\{\varphi_{\alpha}(i), \varphi_{\alpha}^{*}(i)\}] = \sum_{ij\alpha} t_{ij}\varphi_{\alpha}^{*}(i)\varphi_{\alpha}(j) + \frac{1}{2}\sum_{ijkl\alpha\beta} \tilde{v}_{ij,kl}\varphi_{\alpha}^{*}(i)\varphi_{\beta}^{*}(j)\varphi_{\alpha}(k)\varphi_{\beta}(l)$$
(15)

Therefore, we see that the energy obtained by making the expectation value of a Hamiltonian with a Slater determinant becomes a functional of the one-body density. Then, we deduce the functional scheme:

$$\{\varphi_{\alpha}, \varphi_{\alpha}^{*}\} \Longrightarrow \rho \Longrightarrow E_{\rm HF}[\rho] \tag{16}$$

 $^{3}$  Here we have used the short-hand notation:

$$t_{ij} = \langle i|T|j\rangle, \quad \tilde{v}_{ij,kl} = \langle ij|\tilde{v}|kl\rangle, \cdots$$

and the fact that  $\tilde{v}_{ij,kl} = -\tilde{v}_{ij,lk}$ .

where  $X \Longrightarrow Y$  means that from X we can get Y.

The Hartree-Fock ground state is finally obtained by minimizing the energy in the space of Slater determinant. This minimization can be achieved by using the Rayleigh-Ritz variational principle:

$$\delta \left[ \langle \Phi | H | \Phi \rangle - E \langle \Phi | \Phi \rangle \right] = 0 \tag{17}$$

where the variation is made on all possible variations of single-particle components. It turns out that the variational principle can be eventually directly formulated either in terms of variation of the one-body density or in terms of single-particle states as(Ring and Schuck book (1980), Blaizot and Ripka book (1986)):

• One-body density variational principle:

$$\delta \left[ E_{\rm HF}[\rho] - \Lambda {\rm Tr}(\rho^2 - \rho) \right] = 0 \tag{18}$$

Here, the right-hand side constraint has been added to insure that the density has only occupation probability equal to 0 or 1. Note also that the properties of the one-body density has to be taken into account to avoid the redundancy in the variation.

• Single-particle variational principle: Equivalently, the energy can be minimized by all possible independent variations of the single-particle components  $\{\varphi_{\alpha}(i), \varphi_{\alpha}^{*}(i)\}$ . Such a variation should however be made by imposing that single-particle states are normalized<sup>4</sup>. This is generally achieved by adding a set of Lagrange multiplier during the minimization leading to a new function to minimize:

$$\delta \left[ E_{\rm HF}[\{\varphi_{\alpha}(i), \varphi_{\alpha}^{*}(i)\}] - \sum_{\alpha} \varepsilon_{\alpha} \Big(\sum_{i} \varphi_{\alpha}^{*}(i)\varphi_{\alpha}^{*}(i) - 1\Big) \right]$$
(19)

To illustrate variational techniques, let us consider the last case. At the minimum, any variation of one of the single-particle state component of the form:

$$\varphi_{\alpha}^{*}(i) \to \varphi_{\alpha}^{*}(i) + \delta \varphi_{\alpha}^{*}(i)$$

should give  $\delta E = 0$ . Making explicitly the variation, one directly deduces:

$$\sum_{j} t_{ij}\varphi_{\alpha}(j) + \sum_{jkl\alpha\beta} \tilde{v}_{ij,kl}\rho_{lj}\varphi_{\alpha}(k) - \varepsilon_{\alpha}\varphi_{\alpha}(i) = 0$$
<sup>(20)</sup>

If we now introduce the mean-field Hamiltonian  $h_{\rm MF}$  defined as <sup>5</sup>:

$$h_{\rm MF}[\rho] = t + Tr_2(\tilde{v}_{12}\rho_2) \tag{21}$$

$$= t + U_{\rm MF} \left[ \rho \right] \tag{22}$$

$$\langle i|Tr_2(\tilde{v}_{12}\rho_2)|k\rangle = \sum_j \langle ik|\tilde{v}_{12}\rho_2|kj\rangle = \sum_{jl} \langle ik|\tilde{v}_{12}|kl\rangle\rho_{lj}$$

<sup>&</sup>lt;sup>4</sup> Note that, one should a priori impose, the orthogonality of the single-particle states. This could be done, but will complicate the derivation.

<sup>&</sup>lt;sup>5</sup> Here, the partial trace on the second particle has been introduced. For instance:

where  $U_{\rm MF}$  denotes the mean-field one-body potential. We see that the minimization of the energy leads to an eigenvalue problem:

$$h_{\rm MF}[\rho]|\varphi_{\alpha}\rangle = \varepsilon_{\alpha}|\varphi_{\alpha}\rangle \tag{23}$$

and that the Lagrange multipliers  $\varepsilon_{\alpha}$  can be interpreted as single-particles energies. At that point there are few important remarks:

• In the Hartree-Fock theory, the original many-body problem is replaced by a much simpler one-body problem. The single-particle states are chosen by selecting the N lowest eigenstates of  $h_{\rm MF}$ . The energy of the last occupied level is called the Fermi energy (see illustration).



FIG. 8: Illustration of the Hartree-Fock theory. Particles occupy levels up to the fermi energy. Below the Fermi energy, the occupation numbers are equal to 1 while above they are equal to 0.

- In the Hartree-Fock single-particle basis, the one-body density and Hartree-Fock hamiltonian are both diagonal and similarly to  $\rho$ , the mean-field hamiltonian writes  $h_{\rm MF}[\rho] = \sum_{\alpha=1}^{N} |\varphi_{\alpha}\rangle \varepsilon_{\alpha} \langle \varphi_{\alpha}|$
- The equation to solve depends on the density and specific numerical methods should be used. There are however two major differences:
  - 1. The single-particle potential  $U_{\rm MF}$  has to be evaluated self-consistently. Indeed, it depends explicitly on the one-body density that itself depends on the single-particle states that are determined using the potential. This could be expressed using the sequence:

$$\{\varphi_{\alpha}\} \Longrightarrow \rho \Longrightarrow U_{\mathrm{MF}}[\rho] \Longrightarrow \{\varphi_{\alpha}\} \Longrightarrow \cdots$$
 (24)

Contrary to usual Schroedinger equation, a self-consistent approach needs to be solved iteratively. The iterative procedure is illustrated in Fig. 9

2. A second difficulty comes from the fermionic nature of the particles that leads to non-local potential. Indeed, let us assume that the basis used to express the mean-field correspond to the position basis, i.e.  $\{|i\rangle\} = \{|\mathbf{r}\rangle\}$ . In the following, we assume that the two-body interaction is local and eventually finite range, i.e.

$$\langle \mathbf{r}_1 \mathbf{r}_2 | v | \mathbf{r}_3 \mathbf{r}_4 \rangle = \delta_{\mathbf{r}_1 \mathbf{r}_3} \delta_{\mathbf{r}_2 \mathbf{r}_4} v(\mathbf{r}_1 - \mathbf{r}_2)$$
(25)

Eq. (23) becomes

$$-\frac{\hbar^2}{2m}\Delta\varphi_{\alpha}(\mathbf{r}) + U_{\rm H}(\mathbf{r})\varphi_{\alpha}(\mathbf{r}) + \int d\mathbf{r}' U_{\rm ex}(\mathbf{r},\mathbf{r}')\varphi_{\alpha}(\mathbf{r}') = \varepsilon_i \varphi_{\alpha}(\mathbf{r})$$
(26)



FIG. 9: Illustration of the practical way to solve self-consistent Hartree-Fock equation. First one has to choose a set of single-particle states that are supposed to not be too far from the solution. Then, from them, the mean-field hamiltonian is computed. By diagonalizing this hamiltonian, new single-particle states are found. Then, the procedure is iterated until the convergence is achieved.

where  $U_{\rm H}$  and  $U_{\rm ex}$  denote respectively the Hartree (Direct) and exchange contribution to the mean-field potential and are given respectively by:

$$U_{
m H}(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r} - \mathbf{r}') 
ho(\mathbf{r}', \mathbf{r}')$$
  
 $U_{
m ex}(\mathbf{r}, \mathbf{r}') = -v(\mathbf{r} - \mathbf{r}') 
ho(\mathbf{r}, \mathbf{r}')$ 

The exchange term is a direct consequence of the Fermi statistic. As could be seen from Eq. (26), this leads to non-local equation for the wave-functions, i.e. the Schrödinger equation verified by  $\varphi_{\alpha}(\mathbf{r})$  depends on its value at all other positions  $\varphi_{\alpha}(\mathbf{r}')$ . Non-local equation are much more complex to solve. As we will see latter, the use of contact interactions with  $v(\mathbf{r}_1 - \mathbf{r}_2) \propto \delta(\mathbf{r}_1 - \mathbf{r}_2)$  leads to similar functional.

## D. Failure of the Hartree-Fock approach: the infinite nuclear matter case

From previous discussion, we see that the nuclear Hamiltonian has the general form:

$$H_{\rm nuc} = \sum_{i} \frac{p^2(i)}{2m} + \sum_{i < j} v_{NN}^{(2)}(i,j) + \sum_{i < j < k} v_{NNN}^{(3)}(i,j,k) + \cdots$$
(27)

One can then use the Hartree-Fock machinery discussed above to obtain an independent particle approximation of the nuclear many-body problem, i.e. :

$$H_{\rm nuc} \Longrightarrow \sum_{i} \left( \frac{p^2(i)}{2m} + V(i) \right) = \sum_{i} h_{\rm MF}(i)$$
(28)

Here, we will consider the so-called "symmetric infinite nuclear matter" case. This ideal infinite case has been introduced as an ideal limiting case when the number of nucleons goes to infinity.

#### 1. Infinite nuclear matter

In nuclei, it is observed that the local density  $\rho(r)$  is almost constant at the center of the nucleus along the nuclear chart (see illustration 2) and equal to  $\rho_0 \simeq 0.16/0.17$  fm<sup>-3</sup>. This properties is known as the saturation properties of nuclei.

In addition, if one consider a nucleus with N neutrons and Z protons, the central neutron and proton densities, resp. denoted by  $\rho_n$  and  $\rho_p$  with  $\rho_0 = \rho_n + \rho_p$ , one has approximately:

$$\frac{\rho_n}{\rho_p} \simeq \frac{N}{Z}.$$
(29)

Having this property in mind, observations in finite systems have been extended to the case where the number of nucleons becomes infinite. Then the density is defined as the number of nucleons A per unit volume, denoted by V:  $\rho = A/V$  (with A= N+Z) while keeping  $\rho_n/\rho_p$  constant. Note that the Coulomb interaction, that would lead to unbound system as Z increases, is removed in that case. Therefore, the main effect coming of the isospin, stems from the Pauli principle, i.e. from the fact that two neutrons cannot occupy the same state while one proton and one neutron can. Two special case are generally retained as test cases:

• The symmetric nuclear matter case: where the number of proton equals the number of protons. Then, we have

$$\rho_n = \rho_p = \frac{\rho}{2}$$

• The neutron matter: where simply Z = 0 leading to  $\rho_p = 0$  and  $\rho_n = \rho$ .

In Figure 10 (left), the energy of symmetric and neutron matter is shown as a function of the density. This curve is generally called Equation Of State (EOS) at zero temperature. In this figure, we see that only symmetric nuclear matter present a stable minimum (shown by a square) called saturation point at density  $\rho_0 \simeq 0.16/0.17$  fm<sup>-3</sup> and energy  $E/A \simeq 16$  MeV.

#### 2. Hartree-Fock theory in infinite systems

Here, we concentrate on the symmetric case, in this case, since the Coulomb interaction is neglected, proton and neutrons are degenerated.

a. Single-particle wave-functions: Let us be here more specific and precise the wave-function for infinite systems. In this case, it is convenient to work in momentum space and use periodic conditions. This means that we cut the systems into identical boxes of volume V and assume periodic boundary conditions. Let us assume three-dimensional boxes of length L (with  $V = L^3$ ). Because of the periodic condition, a convenient basis for the problem, is provided by plane waves written as:

$$\langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{V^{1/2}} e^{i \mathbf{p} \mathbf{r}/\hbar} = \frac{1}{V^{1/2}} e^{e^{i(k_x x + k_y y + k_z z)}}$$
 (30)

where  $\mathbf{p} \equiv \hbar \mathbf{k}$  and where the boundary conditions impose:

$$k_i = \frac{2\pi n_i}{L}, \quad i = x, y, z, \quad n_i = 0, \ \pm 1, \ \pm 2, \cdots$$
 (31)

Let us denote by A the number of particles in the finite volume V. The infinite system limit has to be understood as the limit  $A \to +\infty$  and  $V \to +\infty$  while keeping  $\rho = A/V$  =cte.



FIG. 10: Left: (Color online) Illustration of the expected behavior of the energy of infinite nuclear matter as a function of the density. The neutron matter is shown by open squares while symmetric nuclear matter is displayed by filled circles. Right: (Color online) Example of Hartree-Fock (black) and Hartree-Fock + perturbation theory (red area) obtained using bare two-body and three-body interaction for symmetric nuclear matter energy at various density. The square indicates the physical position of the saturation point around  $\rho \simeq 0.16 \text{ fm}^{-3}$  and  $E/A \simeq -16$  MeV. According to eq. (35), a density of 0.16 fm<sup>-3</sup> leads to  $k_F \simeq 1.33$  fm<sup>-1</sup>.

b. Independent particle states: Thanks to the translational invariance, any eigenstate of a one-body hamiltonian in this case identify with the plane-wave given by equation (30). Including the fact that nucleons have spins and isospin, in the following, single-particle states are written as  $\varphi_{\mathbf{p},\sigma,\tau}(\mathbf{r})$ . Then, sums over single-particle states presented previously in a rather general manner now becomes:

$$\sum_{i} \cdots \implies \sum_{\tau\sigma} \int_{\mathbf{p}} d^{3}\mathbf{p} \cdots = \frac{V}{(2\pi)^{3}} \sum_{\tau\sigma} \int_{\mathbf{k}} d^{3}\mathbf{k} \cdots$$
(32)

where the first sum runs over spin up and spin down as well as over proton and neutrons.

In the Hartree-Fock approximation, the Slater determinant is obtained as a product of plane waves with momentum lower than a maximal value  $|p| < |p_F|$  where  $|p_F|$  corresponds to the Fermi momentum. The density can be expressed as a function of the Fermi energy through  $\varepsilon_F = \hbar^2 k_F^2/(2m)$ . The one-body density (in different spin and isospin channels) then takes the form:

$$\rho_{\sigma,\tau} = \frac{V}{(2\pi)^3} \int_{\mathbf{k}} d^3 \mathbf{k} |\mathbf{k}\sigma\tau\rangle n_{\sigma\tau}(\mathbf{k}) \langle \mathbf{k}\sigma\tau|$$
(33)

where  $n_{\sigma\tau}(\mathbf{k}) = 1$  for  $k \leq k_F$  and zero elsewhere<sup>6</sup>. Starting from the above density, one could obtain the neutron or proton densities by summing on different spins, while summing also on the isospin gives the total density, i.e.  $\rho = \sum_{\sigma\tau} \rho_{\sigma\tau}$ .

<sup>&</sup>lt;sup>6</sup> Note that here, because we consider the symmetric nuclear matter case, the proton and neutron Fermi momentum are identical. In general, they are different from each others.

The density is directly connected to the Fermi momentum. Indeed, we have:

$$A = \operatorname{Tr}(\rho) = \sum_{\sigma,\tau} \operatorname{Tr}(\rho_{\sigma\tau}) = \frac{V}{(2\pi)^3} \sum_{\tau\sigma} \int_{\mathbf{k}} d^3 \mathbf{k} n_{\sigma\tau}(\mathbf{k})$$
$$= \frac{4V}{(2\pi)^3} \int_0^{k_F} 4\pi k^2 dk = \frac{2V}{3\pi^2} k_F^3$$
(34)

where the factor 4 comes from the spin-isospin degeneracy. Noting that  $\rho = A/V$  we finally obtain:

$$\rho = \frac{2}{3\pi^2} k_F^3 \tag{35}$$

A density of 0.16 fm<sup>-3</sup> leads to  $k_F \simeq 1.33$  fm<sup>-1</sup>.

The kinetic energy can equivalently be obtained using the same technique:

$$E_{\rm kin} = \left\langle \frac{p^2}{2m} \right\rangle = \frac{V}{(2\pi)^3} \int_{\mathbf{k}} d^3 \mathbf{k} \frac{\hbar^2 \mathbf{k}^2}{2m} n_{\sigma\tau}(\mathbf{k}) = \frac{\hbar^2}{2m} \frac{4V}{(2\pi)^3} \int_0^{k_F} 4\pi k^4 dk = \frac{\hbar^2}{m} \frac{V}{5\pi^2} k_F^5 = A \frac{\hbar^2}{m} \frac{1}{5\rho\pi^2} k_F^5$$
(36)

From which we deduce that the kinetic energy per particle is given by:

$$\frac{E_{\rm kin}}{A} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} = \frac{3}{5} \varepsilon_F = \frac{3}{5} \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\rho\right)^{2/3}$$
(37)

Note that this expression illustrates that the kinetic energy becomes a functional of the density. Similarly, given a two-body and/or three-body interaction, an explicit form of the mean-field Hamiltonian can be obtained in momentum space (not described here).

An illustration of result obtain with modern nucleon-nucleon interaction including the three-body interaction is given in right side of Figure 10 (black curve). The open square indicates the saturation point. While the Hartree-Fock approximation leads also to a saturation, the equilibrium is far from the expected value. For instance, the energy at the minimum is around 8 MeV/A and therefore accounts only for 50 % of the binding. It is indeed well known that Hartree-Fock only starting from the bare nucleon-nucleon interaction is a poor approximation. This indicates that effects beyond Hartree-Fock are important. To treat this effect, one needs to introduce a residual interaction such that:

$$H_{\rm nuc} = \sum_{i} h_{\rm MF}(i) + V_{\rm res} \tag{38}$$

where by definition  $V_{\rm res}$  includes all what has not been accounted for in the mean-field part. The treatment of  $V_{\rm res}$  requires many-body techniques (that are out of the scope of present lectures) that are much more involved than the independent particle approach. Then, the correlated ground state will be a mixing of the original state as well as of different 2particles-2holes, 3p-3h,... excitations. The result of such a perturbation calculation is given in Figure 10 leading to a much better agreement with the expected saturation point.

### **III. DENSITY FUNCTIONAL THEORY FOR NUCLEI**

In view of the preceding discussion, we are facing the following dilemma: many aspects of nuclei can be fairly well understood assuming that nucleons behaves like independent particles

moving in an external one-body field. Unfortunately, the natural approach starting from the nuclear hamiltonian, i.e. the Hartree-Fock theory, to map a many-body problem into a onebody theory does not work in nuclear physics. Guided by the relative simplicity emerging from experimental observation, nuclear physicist have introduced the nuclear Energy Density Functional (EDF) concept. The EDF is very close in spirit to the Density Functional Theory (DFT) introduced in electronic systems. In such theories, similarly to the Hartree-Fock (HF) case, the initial many-body problem is replaced by a simpler one-body problem and can also be depicted by figure 6. However, DFT is conceptually completely different from HF. Indeed, while HF is an approximation of the nuclear many-body problem starting from the Hamiltonian, DFT/EDF goal is to provide an exact reformulation of the initial problem and can be regarded as an *ab-initio* approach. In particular, its minimal goal is to provide a ground state energy and one-body local density as close as possible to the observed one and therefore it incorporates effects much beyond the pure HF approach. Below, a discussion of some connections connections and differences DFT in electron and EDF in nuclei is given. In this section mainly general concepts are presented and those who are directly interested in EDF from a simpler perspective can directly jump to section III B

#### A. DFT versus EDF: common aspects and differences

The nuclear EDF has many aspects in common with the DFT theory. DFT is a very powerful approach that can be applied to a wide range of physical problems. A complete description of all the ramifications of DFT is certainly out of the scope of the present document (for details see excellent the textbooks (Paar and Yang, book (1989), Dreizler and Gross, book (1990), Koch and Holthausen, book (2001), Fiolhais et al, book (2003)). Nevertheless, to understand connections between EDF and DFT a brief overview of DFT is given below.

#### 1. Selected aspects of DFT

At first sight, Density Functional Theory might appear as a nice trick to find properties like the ground state energy, the local density of a complex system of interacting electrons without solving the associated N-body problem. In reality, "Density functional theory is a completely different, formally rigorous, way of approaching any interacting problem, by mapping it exactly to a much easier-to-solve non-interacting problem". Some of the theorems and aspects of DFT relevant for the present discussion are listed below:

- Hohenberg-Kohn theorem: The DFT concept has been introduced to describe electrons interacting through the well known repulsive *Coulomb interaction* and *bound* by the surrounding Ions. The starting point is the Hohenberg-Kohn (HK) theorem (Hohenberg and Kohn, Phys. Rev. 136 (1964)): The HK theorem demonstrates that the problem of interacting electrons in an external field (surrounding ions) can be replaced by a problem where the energy is replaced by a functional of the local density. Eventually, in some cases (v-representability), the complex interacting system can be replaced by an ensemble of non-interacting electrons in a local external field  $v(\mathbf{r})$ . This potential can be written as a functional of the local density  $n(\mathbf{r}) \equiv \rho(\mathbf{r}, \mathbf{r})$ . At the minimum of the functional, the energy of the non-interacting system matches the energy of the interacting one and the local density matches the local density of the exact ground state.
- Kohn-Sham state and equation: Kohn-Sham introduced the notion of auxiliary state (Kohn and Sham, Phys. Rev. 140 (1965)). In the KS approach, a Slater determinant denoted by  $\Phi$  is introduced to compute the local density (see also discussion in

Perdew et al, Phys. Rev. B23 (1981)). Associated single-particle states (Kohn-Sham orbitals), denoted by  $\varphi_{\alpha}$  are solution of the Kohn-Sham equation:

$$\left\{-\frac{\hbar^2 \nabla^2}{2m} + v(\mathbf{r})\right\} \varphi_{\alpha}(\mathbf{r}) = \varepsilon_i \varphi_{\alpha}(\mathbf{r}).$$
(39)

Note that the auxiliary state itself has no specific physical meaning. This leads to the following sequence of mapping:

$$\Phi = \mathcal{A}(\{\varphi_{\alpha}\}_{\alpha=1,N}) \Longrightarrow n(\mathbf{r}) \Longrightarrow v(\mathbf{r}) \Longrightarrow \mathcal{E}[n(\mathbf{r})] \Longleftrightarrow E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$
(40)

- Construction of the functional: The difficulty of course is to construct the "exact" functional. Many techniques and degrees of approximation to it have been proposed, starting from the Local Density approximation (LDA), where the functional depends only on the local density, to the Gradient Expansion Approximation (GEA), Generalized Gradient Approximation (GGA), to Meta-GGA, where different orders of density gradients are introduced progressively (Fiolhais et al, book (2003)). Note that alternative methods like Optimized Effective Potential (OEP) are also extensively used.
- Additional theorems and extensions: Starting from the pioneering work of Hohenberg, Kohn and Sham, many theorems useful in DFT have been proven. Some of them are specially related to the discussion on EDF are quoted below:
  - Density Matrix Functional Theory (DMFT): Gilbert (Gilbert Phys. Rev. B12 (1975)) has shown that the one-body density matrix (OBDM)  $\rho(\mathbf{r}, \mathbf{r}')$  can be used instead of the local density to construct the functional. The functional can equivalently be written either in terms of the OBDM or in terms of occupation numbers  $n_{\alpha}$  and natural orbitals  $\varphi_{\alpha}$ . One of the advantages of this approach, compared to the Kohn-Sham scheme, is that single-particle states and occupations identify with the exact ones at the minimum, and therefore carry the information on all one-body degrees of freedom.
  - Pairing: DFT has been generalized to account for pairing correlations in ref. (Oliveira et al, Phys. Rev. Lett. 60 (1988)).
  - Time-Dependent Density-Functional Theory (TDDFT): The possibility to describe non-equilibrium dynamics of electrons has been initiated by the Runge-Gross (RG) theorem (Runge and Gross, Phys. Rev. Lett. 52 (1984)). The proof of the theorem has shown in particular that the current vector  $\mathbf{j}(\mathbf{r})$ should also be introduced and that the functional for time-dependent process might be highly non-local in time.
  - Excited states: Using a generalization of the Rayleigh-Ritz theorem given in, the Ensemble Kohn-Sham theory has been proposed to access not only the ground state but also excited states (Gross et al, Phys. Rev. A37 (1988)). Note that TDDFT is nowadays a tool of choice to get information on excited states.

## 2. Selected aspects of EDF

A detailed description of various aspects related to EDF will be given in the following. The goal of the present section is to introduce some of the important features of what is nowadays called Energy Density Functional. These features are introduced in order to follow as much as possible the concepts introduced for DFT in section III A 1 and underlines resemblances and differences.

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- EDF for nuclei: The EDF concept has been introduced to describe nucleons in nuclei interacting through the *strong nucleon-nucleon interaction*. Contrary to electronic systems, nuclei are *self-bound* systems for which the original HK theorem does not apply. In its simplest form, the EDF theory corresponds to the replacement of the initial complex many-body problem by a energy functional of the density. Historically, the EDF theory has been empirically introduced in the 70's without relying on a firm theorem. However, recently, theorems for self-bound systems have been proven where the laboratory density is to be replaced by the density in the intrinsic frame (see Messud et al, Phys. Rev. C80 (2009) and refs. therein).
- Single-Reference EDF and symmetry breaking: in its simplest form, called hereafter Single-Reference (SR)-EDF, similarly to DFT, an auxiliary (Reference) state is introduced to construct the different quantities entering in the functional. When pairing is neglected, the reference state is a Slater determinant. When pairing is included, a quasi-particle vacuum is constructed (written generically as  $|\Phi\rangle = \prod \beta_i |-\rangle$ below). Observables (normal and anomalous densities, gradients of the densities ...) entering in the functional are denoted generically by  $\{\langle A_{\alpha} \rangle\}$ . SR-EDF can then be schematically represented by the sequence:

$$|\Phi\rangle = \prod \beta_i |-\rangle \Longrightarrow \langle A_\alpha \rangle \implies v(\langle A_\alpha \rangle) \implies \mathcal{E}_{\text{EDF}}[\langle A_\alpha \rangle] \iff E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$
(41)

Two important remarks are in order. First, properties of the auxiliary state like singleparticle energies are often used to get physical insight in nuclei. However, having in mind the strict density functional theory framework, it is to be clarified if the auxiliary state could be used to get such physical information. Second, an important aspect of the SR-EDF level is to use reference states that explicitly break some symmetries of the original bare Hamiltonian. Allowing the reference state to break the symmetries is a way to incorporate *static* long-range correlations associated with collective modes, as for example deformation and pairing, with very moderate effort. However, the breaking of symmetries (translational, rotational, parity, particle number, to name the most common ones) forbids a trivial connection of the nuclear SR-EDF formalism to the original existence theorems. Indeed, the density that minimizes the exact HK energy functional must reflect the symmetries of the exact ground state of the system. In fact, the appearance of symmetry-breaking solutions in nuclear EDF calculations underlines two important elements (i) it is crucial and numerically not too difficult to grasp the most important *static* correlations using rather simple approximate functionals and a single-determinantal reference state (ii) kinematic correlations associated with the corresponding symmetry modes (Goldstone modes) as well as the correlations due to the fluctuation of their order parameters are extremely difficult to incorporate into a single-determinantal approach. In other words, correlations associated with highly non-local processes such as large-amplitude collective motions can hardly be described within a SR approach based on a standard, nearly-local EDF. Last, it is important to keep in mind that broken symmetries like pairing or deformation are directly observed experimentally for instance in odd-even mass effects or through the observation of rotational bands.

• Effective interaction and Construction of the SR-EDF functional: current EDF used are mainly based on zero-range (Skyrme like) or finite range (Gogny like) effective interactions. The use of zero range Skyrme interaction (Skyrme, Phil. Mag, 1 (1956)) has been originally proposed to obtain a functional form in (Vautherin and Brink, Phys. Rev. C5 (1972)). In this reference, starting from the Skyrme interaction including three-body forces, the Hartree-Fock approximation is used to get a functional

of the local density  $\rho$ , the kinetic density  $\tau$ , etc. Parameters of the functional have then been directly adjusted on specific properties of infinite nuclear matter (energy, saturation density and incompressibility) and finite nuclei. Due to the use of effective interactions and many-body techniques very similar to HF or HFB, EDF are sometimes themselves confused with HF or HFB theory which might be misleading. A list of reason why the EDF should not be mixed with such theories are given below:

- ♦ Original Skyrme interaction, restricted to two and three-body terms, do not provide a proper description of nuclear systems close to the saturation point. For this reason, density dependent effective interactions have been introduced. Strictly speaking, one cannot speak anymore about a Hamiltonian and Hartree-Fock approximation if the underlying interaction depends itself on the trial state on which it is applied.
- $\diamond$  The exchange term in the Coulomb interaction is rarely treated exactly and most often the Slater approximation is made (see below).
- $\diamond$  When pairing is included, different effective interaction are often used in the mean-field and pairing channels respectively, showing that the very notion of an underlying Hamiltonian on which the Hartree-Fock approximation is made does not exist.
- ♦ In practice the functional parameters are directly adjusted on experimental observations. Since experiments include complex correlations in nuclei, one expect that coefficients contain much more physics than the simple Hartree-Fock approximation made with the bare nuclear Hamiltonian.

These are few examples emphasizing the difference between HF and EDF. Obviously, one can eventually continue to use terminology like "Skyrme HF" but things might become very confusing in the near future. Indeed, with new soft interactions, it is now possible to make the true HF approximation of the vacuum nuclear Hamiltonian. This HF approximation has nothing to do with EDF theory. In this lecture, SR-EDF will be systematically used to not confuse with the HF theory.

Finally, it is important to realize that there are several advantages in constructing a functional from an effective interaction. EDF deduced in this way are very rich and automatically contain many density dependent terms as well as term depending on gradients... of the density. As a direct consequence, even original EDF can already be classified at least as a Meta-GGA approach. In addition, time-odd terms as well as specific combinations of terms that automatically ensure some physical properties like Galilean invariance, naturally appear in the functional.

- Extensions: Similarly to DFT many extensions of SR-EDF have been proposed:
  - Density Matrix Functional Theory (DMFT): Following the idea of Gilbert, the possibility to enrich the functional by using functional of the one-body density matrix (OBDM) or occupation numbers  $n_{\alpha}$  and natural orbitals  $\varphi_{\alpha}$  has been recently rediscussed (Papenbrock et al, Phys. Rev. C 75 (2007), Lacroix, Phys. Rev. C79 (2009)). DMFT might in particular be a way to conciliate the physical interpretation of single-particle energies used in EDF since in that case singleparticle states are meaningful and should be identified with the exact natural orbitals.
  - Pairing: As mentioned above, pairing correlations are often included by considering functionals not only of the normal density but also of the anomalous density (see for instance (bender et al, Rev. Mod. Phys. (2003))).

- Time-Dependent Energy Density Functional (TD-EDF): Right after first applications of EDF to study static properties of nuclei, the dynamics of nuclei using TD-EDF has been developed (Bonche et al, Phys. Rev. C13 (1976)).
- Restoration of broken symmetries and Multi-Reference EDF (MR-EDF): At the SR-EDF level several symmetries are explicitly broken (see discussion above). In a Hamiltonian case, those symmetries could be restored through configuration mixing using the Generator Coordinate Method (GCM) (Ring and Schuck, book (1980)). Guided by the Hamiltonian case, configuration mixing techniques are nowadays used to incorporate correlations associated with large amplitude collective motion beyond the static ones. In that case, a new many-body state, denoted by  $|\Psi\rangle$  and written as

$$|\Psi\rangle = \sum_{Q} f_{Q} |\Phi(Q)\rangle \tag{42}$$

is introduced, where  $|\Phi(Q)\rangle$  corresponds to a set of reference states function of some collective parameters  $Q = \langle Q \rangle$ . Configuration mixing within EDF, called hereafter Multi-Reference EDF, is not only used to restore symmetry but also provides a tool of choice to access excited states of the nucleus. Recent studies (Dobaczewski et al, Phys. Rev. C 76 (2007), Lacroix et al, Phys. Rev. C79 (2009), Bender et al, Phys. Rev. C79 (2009), Duguet et al, Phys. Rev. C79 (2009)) have pointed out some deficiencies in combining functional theory and configuration mixing technique as well as the necessity to develop a clear theoretical framework for MR-EDF approach (see discussion below).

## B. EDF from a simple perspective

The main challenge in EDF is to design a functional of the density able to describe the whole nuclear chart. The strategy followed in nuclear physics, that starts with effective interaction is very specific. Before, discussing this strategy, I will present two examples illustrating the EDF concept from a simpler perspective.

#### 1. Simple illustration for EDF in infinite nuclear matter

To illustrate how EDF works in nuclear physics, let us consider again the infinite nuclear matter case. We have seen previously that the Hartree-Fock theory cannot describe the energy of infinite systems and effects much beyond HF are required. We now consider the same problem from a density functional point of view using the following steps:

- 1. We first introduce an independent particle many-body Slater determinant relevant for the considered problem. For nuclear matter, this state is the same as for the HF case (see section II D 2)
- 2. From the Slater determinant, we then construct the density. In the infinite nuclear matter, the density is constant and denoted by  $\rho$ .
- 3. Then, the main challenge is to guess the functional itself, i.e.  $E = \mathcal{E}(\rho)$  such that it provides a correct description of the system at the minimum. We write the functional as:

$$\mathcal{E}(\rho) = \mathcal{E}_{\rm kin}(\rho) + \mathcal{E}_{\rm pot}(\rho) \tag{43}$$

 $\mathcal{E}_{kin}(\rho)$  correspond to the kinetic energy estimated with a Slater determinant. Its form has been derived previously and is given by Eq. (37). As an illustration of simple functional, we consider here that the other term writes as a polynomial of  $\rho$ :

$$\mathcal{E}_{\text{pot}}(\rho) = a_1 \rho + a_2 \rho^2 + \cdots \tag{44}$$

4. Generally, the functional is adjusted either on experimental observation or some reference curves or both. In the present case, the curve obtained in infinite systems from ab-initio calculation is used. An illustration of a fit obtained with a fifth order polynomial is shown in Figure 11.



FIG. 11: (Color online) Consider a reference curve that gives the energy of symmetric nuclear matter as a function of its density (red line). The goal is to fit the curve by energy written as a functional of the density of an independent particle state. The first step is to write the functional as a sum of the kinetic and potential energy term. For independent particle system, the kinetic term directly express as a functional of  $\rho$ . As an illustration, it is assumed here than the potential part  $\mathcal{E}_{pot}(\rho)$  simply writes as a polynomial of the density. It is straightforward to show that a fit (blue circles) with a fifth order polynomial gives a perfect reproduction of the curve.

This simple example illustrates the interesting feature of functional theories, on one side the simplicity of independent particle theory is kept while on the other side correlation much beyond the pure Hartree-Fock theory are treated in a simple way. Indeed, by fitting directly coefficients of the functional on observables that contains all the correlations, the functional theory itself goes much beyond Hartree-Fock framework. Indeed, while pure HF in nuclear matter leads to more than 50% error on the binding energy, the functional theory cannot be distinguished from the reference curve. EDF or DFT are very powerful theories.

The introduction of EDF in nuclear system in the early 70's was a major breakthrough. Because of the use of effective interaction (Skyrme or Gogny like), the nuclear EDF is strongly guided by the Hartree-Fock framework. In the following, the validity of independent particle picture in nuclei will be further discussed. Actual strategy to design EDF starting from effective two-body interaction will be explained.

#### 2. Simple illustration of EDF in finite systems

As illustrated in the introduction, nuclear density profiles and effective potentials have very specific shapes with constant values inside the nucleus and sharp surface (equations (4) and (2)). One sees that a fairly good approximation would be given by:

$$V(r) = \frac{V_0}{\rho_0} \rho(r) = c_0 \rho(r)$$
(45)

and therefore the one-body potential directly becomes a functional of the density. Assuming that this potential can be deduced from the derivative of the energy with respect to the local density, i.e.  $V(r) = \frac{\partial \mathcal{E}_{\text{pot}}[\rho]}{\partial \rho(r)}$ , one can finally express the potential part of the EDF energy as:

$$\mathcal{E}_{\rm pot} \propto \frac{1}{2} c_0 \int \rho^2(r) dr.$$
 (46)

Further improvement of the functional can be made along this empirical line. For instance, assuming that the spin-orbit component is mainly a surface effect and that  $V_{\text{S.O.}} \propto \nabla V(r)$ ls, one directly get that the spin-orbit becomes a functional of the density gradient.

Instead of using the above method, the functional form of the energy is often introduced by making use of effective forces like Skyrme or Gogny interaction. Let us now come back to the mean-field Hamiltonian given by Eq. (26). If one neglects the exchange potential and assumes a two-body zero-range interaction:

$$v(\mathbf{r}_1 - \mathbf{r}_2) = c_0 \delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{47}$$

then, the mean-field identifies with the Hartree contribution and reads:

$$U_{\rm H}(\mathbf{r}) = c_0 \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}') = c_0 \rho(\mathbf{r}).$$
(48)

Therefore, a simple interaction given by (47) gives <sup>7</sup> the empirical relationship found previously. Obviously, such interaction cannot be confused with the bare interaction presented in figure 1 and should be understood as an *effective interaction*.

# C. Effective interaction based Energy Density Functional: the Skyrme interaction example

The simple example presented in section III B 2 shows that zero range interactions might provide a suitable effective treatment of nuclei. Obviously, the simple form (47), cannot grasp the full complexity of nuclei. In the 70's, following the original work of Skyrme, EDF based on more general effective interaction with zero range have been introduced. In its most standard form, the effective interaction writes:

 $<sup>^{7}</sup>$  Note that this interaction is sometimes called contact interaction

$$v(\mathbf{r}_{1} - \mathbf{r}_{2}) = t_{0} (1 + x_{0} \hat{P}_{\sigma}) \,\delta(\mathbf{r}) \qquad \text{central term}$$

$$+ \frac{1}{6} t_{3} (1 + x_{3} \hat{P}_{\sigma}) \,\rho^{\alpha}(\mathbf{R}) \,\delta(\mathbf{r}) \qquad \text{density dependent term}$$

$$+ \frac{1}{2} t_{1} (1 + x_{1} \hat{P}_{\sigma}) \left[ \mathbf{P}^{\prime 2} \,\delta(\mathbf{r}) + \delta(\mathbf{r}) \,\mathbf{P}^{2} \right] \qquad (49)$$

$$+ t_{2} (1 + x_{2} \hat{P}_{\sigma}) \,\mathbf{P}^{\prime} \cdot \delta(\mathbf{r}) \,\mathbf{P} \qquad \text{non local terms}$$

$$+ i W_{0} \sigma. \left[ \mathbf{P}^{\prime} \times \delta(\mathbf{r}) \,\mathbf{P} \right] \qquad \text{spin orbit term}$$

where we have used the standard notation:

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \qquad \mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) \qquad \mathbf{P} = -\frac{i\hbar}{2}(\nabla_1 - \nabla_2)$$
(50)

and where

$$\sigma = \sigma_1 + \sigma_2, \qquad P_\sigma = (1 + \sigma_1 \cdot \sigma_2)$$

 $P_{\sigma}$  exchange the spin of the two particles. Note finally that,  $\mathbf{P}'$  is the complex conjugate of  $\mathbf{P}$  acting on the left.

In order to obtain the EDF, the spirit of DFT is followed. An auxiliary Slater determinant  $|\Psi\rangle$  is assumed for the many-body state and the energy is obtained simply by performing the expectation value of the effective Hamiltonian, denoted below as  $H(\rho)$  with the independent particle state (details not shown here). The total energy then reads:

$$\mathcal{E} = \mathcal{E}_{\rm kin} + \mathcal{E}_{\rm sky} + \mathcal{E}_{\rm Coul} \tag{51}$$

where the three terms correspond respectively to the kinetic, Skyrme, and Coulomb part. After lengthy but straightforward calculation, one obtain

$$\mathcal{E} = \langle \Psi | H(\rho) | \Psi \rangle = \int \mathcal{H}(r) d^3 \mathbf{r}$$
(52)

with

$$\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{Coul}}$$
(53)

where  $\mathcal{K} = \hbar^2 \tau / (2m)$  and  $\mathcal{H}_{\text{Coul}}$  correspond to the kinetic and Coulomb part while the other terms are given by:

$$\begin{aligned} \mathcal{H}_{0} &= \frac{1}{4} t_{0} \Big[ (2+x_{0})\rho^{2} - (2x_{0}+1)(\rho_{p}^{2}+\rho_{n}^{2}) \Big] \\ \mathcal{H}_{3} &= \frac{1}{24} t_{3} \rho^{\alpha} \Big[ (2+x_{3})\rho^{2} - (2x_{3}+1)(\rho_{p}^{2}+\rho_{n}^{2}) \Big] \\ \mathcal{H}_{\text{eff}} &= \frac{1}{8} \Big[ t_{1}(2+x_{1}) + t_{2}(2+x_{2}) \Big] \tau \rho \\ &+ \frac{1}{8} \Big[ t_{2}(2x_{2}+1) - t_{1}(2x_{2}+1) \Big] \big( \tau_{p}\rho_{p} + \tau_{n}\rho_{n} \big) \\ \mathcal{H}_{\text{fin}} &= \frac{1}{32} \Big[ 3t_{1}(2+x_{1}) - t_{2}(2+x_{2}) \Big] (\nabla \rho)^{2} \\ &- \frac{1}{32} \Big[ 3t_{1}(2x_{1}+1) + t_{2}(2x_{2}+1) \Big] \big[ (\nabla \rho_{p})^{2} + (\nabla \rho_{n})^{2} \big] \\ \mathcal{H}_{\text{so}} &= \frac{1}{2} W_{0} \Big[ \mathbf{J} . \nabla \rho + \mathbf{J}_{p} . \nabla \rho_{p} + \mathbf{J}_{n} . \nabla \rho_{n} \Big] \\ \mathcal{H}_{\text{sg}} &= -\frac{1}{16} \big( t_{1}x_{1} + t_{2}x_{2} \big) \mathbf{J}^{2} + \frac{1}{16} \big( t_{1} - t_{2} \big) \Big[ \mathbf{J}_{p}^{2} + \mathbf{J}_{n}^{2} \Big] \end{aligned}$$

where  $\rho = \rho_n + \rho_p$ ,  $\tau = \tau_n + \tau_p$ . We see that the functional not only depends on the density but also on its derivative as well as the kinetic energy density and spin densities defined through:

$$\rho_{q}(\mathbf{r}) = \sum_{i,s} |\varphi_{i,s,q}(\mathbf{r})|^{2}$$
  

$$\tau_{q}(\mathbf{r}) = \sum_{i,s} |\nabla \varphi_{i,s,q}(\mathbf{r})|^{2}$$
  

$$\mathbf{J}_{q} = \sum_{i,s,s'} \varphi_{i,q,s'}^{*}(\mathbf{r}) \nabla \varphi_{i,q,s}(\mathbf{r}). \langle s' | \sigma | s \rangle$$
(54)

We also see that the Skyrme functional provides already a much reacher functional than a functional of the density only. While the origin of the functional is motivated by the effective interaction, one can also directly write it as:

$$\mathcal{H}[\rho,\tau,\mathbf{J},\ldots] = \mathcal{K} + C^{\rho\rho}\rho^2 + C^{\rho_p\rho_p}\rho_p^2 + \cdots$$
(55)

without referring to the original set of parameters in the force.

### 1. Illustration of Skyrme EDF in infinite nuclear matter

Let us come back to the infinite nuclear matter case and illustrate how the functional parameter can be adjusted. As we will see, the method is very similar to the illustration given in figure 11. For simplicity, we will neglect here  $\mathcal{H}_{sg}$ .

In the symmetric infinite system with, the densities are constant and verifies  $\rho_p = \rho_n = \rho/2$ ,  $\tau_n = \tau_p = \tau/2$ . Therefore all quantities containing gradients are equal to zero. As a consequence, only  $\mathcal{H}_0$ ,  $\mathcal{H}_3$  and  $\mathcal{H}_{\text{eff}}$  do not cancel out. As in the Fermi gas model, to treat infinite systems, we consider a Slater determinant occupying lowest momentum up to  $k_F$  with periodic boundary condition. Accordingly, densities are constant and the kinetic term is given by Eq. (37). In this case,  $\mathcal{H}(\mathbf{r}) = \mathcal{H}$  becomes independent of  $\mathbf{r}$ . Then, the energy per particle in a volume becomes:

$$\frac{\mathcal{E}}{A} = \frac{1}{A} \int \mathcal{H}(r) d^3 \mathbf{r} = \frac{V}{A} \mathcal{H} = \frac{1}{\rho} \mathcal{H}$$
$$= a_0 \rho^{2/3} + a_1 \rho + a_2 \rho^{5/3} + a_3 \rho^{\alpha+1}$$
(56)

where different coefficients  $a_1$ ,  $a_2$  and  $a_3$  can eventually be expressed in terms of  $t_0$ ,  $x_0$ ,  $t_1$ , ... while

$$a_0 = \frac{3}{5} \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\right)^{2/3} \tag{57}$$

Therefore, while our starting point was an effective interaction, we are left with a functional of the density that should be adjusted on the properties of some reference curves. For infinite systems, instead of fitting directly the whole curve, properties around equilibrium value are generally imposed:

• Equilibrium energy: At equilibrium, the density identify with the saturation density  $\rho_0 = 0.16$  fm<sup>-3</sup> while the energy equals  $E_0/A = -16$  MeV giving:

$$\frac{E_0}{A} = a_0 \rho_0^{2/3} + a_1 \rho_0 + a_2 \rho_0^{5/3} + a_3 \rho_0^{\alpha+1}$$
(58)

• **Pressure:** Since the saturation point should be a minimum, it should verify:

$$\left. \frac{\partial (\mathcal{E}/A)}{\partial \rho} \right|_{\rho = \rho_0} = 0$$

leading to:

$$0 = \frac{2}{3} \frac{a_0}{\rho_0^{1/3}} + a_1 + \frac{5}{3} a_2 \rho_0^{2/3} + (1+\alpha) a_3 \rho_0^{\alpha}$$
(59)

This condition can also be interpreted as the cancellation of the internal pressure at equilibrium. Indeed, in a physical system, the pressure is defined as:

$$P = -\frac{\partial \mathcal{E}}{\partial V}\Big|_{A} = \frac{A}{V^{2}} \left.\frac{\partial \mathcal{E}}{\partial \rho}\right|_{\rho=\rho_{0}} = \rho^{2} \left.\frac{\partial (\mathcal{E}/A)}{\partial \rho}\right|_{\rho=\rho_{0}}$$
(60)

• Incompressibility: One generally also constraint the curvature of equation of state around the minimum, i.e.  $\partial^2 E / \partial^2 \rho$ . This curvature is directly connected to the resistance of the nucleus against compression which is generally discussed in terms of the incompressibility modulus  $K_{\infty}$ , defined through:

$$K_{\infty} = 9\rho_0^2 \left. \frac{\partial^2(\mathcal{E}/A)}{\partial^2 \rho} \right|_{\rho = \rho_0} \tag{61}$$

This coefficient can be extracted from the study of collective motion in nuclei and more specifically the monopole vibration (see below) leading to a typical value  $K_{\infty} = 230 - 270$  MeV. Adding this constraint, one gets a third equation:

$$K_{\infty} = -2a_0\rho_0^{2/3} + 10a_2\rho_0^{5/3} + 9\alpha(1+\alpha)a_3\rho_0^{\alpha+1}$$
(62)

Properties at the saturation points provides three constraint on the different coefficients, while we have 4 unknown quantities. Let us for simplicity assume that  $a_2 = 0$  (which is equivalent to keep only  $t_0$  and  $t_3$  terms in the interaction). Then, the different coefficients can be deduced from the nuclear matter properties. The simple example presented here illustrate the EDF strategy. Nowadays, more complex functional are being used with up to 10 to 20 parameters to adjust. Accordingly, additional constraints should be imposed. Most common are: properties of neutron and asymmetric nuclear matter, semi-infinite system, ground state energy and radius of nuclei and sometimes their shell structure, energies of monopole and quadrupole collective motion.

#### 2. Application in finite nuclei

The main interest of functional based theory is that it is expected to be universal. Once the functional has been found, it could be equivalently be applied to infinite or finite systems. In finite systems, the auxiliary state is a Slater determinant formed from N neutrons and Z protons. The energy of the system takes the form (52). In practice, the single-particle states are obtained by solving the set of equations:

$$h_{MF}[\rho]|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle \tag{63}$$

where the mean-field potential is directly defined from the functional itself through:

$$h_{MF}[\rho]_{ij} = \frac{\partial \mathcal{E}[\rho]}{\partial \rho_{ji}} \tag{64}$$

The mean-field identifies with the standard Hartree-Fock hamiltonian when a bare interaction is used. It should however be kept in mind that the mean-field defined through the derivative of the energy will differ from Eq. (26) used in combination with the Skyrme effective interaction at least due to the presence of density dependent term in the interaction ( $t_3$ term). More generally, EDF are sometimes given without referring to any interaction, then Eq. (64) provides the only way to define a mean-field consistently. The mean-field itself is a functional of the density and its derivatives. Therefore Eq. (63) should be solved iteratively as depicted in figure 9.

Examples of single-particle self-consistent potential as well as associated proton and neutrons level scheme are given in figure 12. We see that the mean-field potential slightly



FIG. 12: (Color online) Example of proton/neutron potentials obtained using Skyrme EDF for  ${}^{40}$ Ca (Z=20) and  ${}^{208}$ Pb (Z=82) nuclei. In each cases, proton and neutron single-particle energies are shown. The length of the line correspond to the degeneracy (2*l* + 1) (Courtesy B. Avez).

differs from the Wood-Saxon potential discussed previously. Nevertheless, the expected gross features of the single-particle potential are recovered. The potential is almost constant and around -50 MeV at the center while it presents a sharp surface. This figure also illustrate the difference between neutron and proton potential. While neutrons only interact through the nuclear field, protons are charged particles and interact with each other through a Coulomb repulsion. In the EDF framework, the Coulomb interaction is also written as a functional of the proton density as:

$$\mathcal{H}_{\text{Coul}}(\mathbf{r}) = \frac{e^2}{2} \rho_p(\mathbf{r}) \int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - \frac{3e^2}{4} \left(\frac{3}{\pi}\right)^{1/3} \rho_p^{4/3}(\mathbf{r})$$
(65)

where the first term correspond to the direct contribution while the second term is an approximation of the exchange term, known as the Slater approximation. It is finally worth to mention that the Fermi energy (the energy of the last occupied state) of proton and neutron is of the order of -10 to -8 MeV for stable nuclei. This however change as the nucleus becomes more neutron rich or more proton rich.

#### 3. Systematic study of nuclear ground state properties

One of the great advantage of nuclear EDF compared to other (supposed exact) methods is its simplicity to implement and its short computation time. Thanks to this advantage, massive comparisons with experimental data over the whole range of the nuclear chart can be made (Bender et al, Rev. Mod. Phys. 75 (2003), ). An illustration of the charge density obtain experimentally and the charge density deduced from the EDF is shown in figure 13 for various nuclei. We see in this figure a very good agreement between the observed and the



FIG. 13: Example of charge density obtained with (e'e') experiments for different nuclei (markers). In each case, corresponding densities starting from two different sets of parameters for the Skyrme interaction are shown (solid and dashed lines correspond resp. to the so-called SkM<sup>\*</sup> and SkX force).

calculated results. For instance, the small oscillation of the central density which is mainly due to the occupancy of s orbitals is rather well accounted for. Similarly, the ground state energy of nuclei that may be as large as few thousand MeV (recall that  $E \simeq 8 \times A$  MeV) is reproduced with a mean deviation of the order of 500 keV. This is illustrated in Figure 14 where the difference between experimental end theoretical binding energy of the nucleus is shown.

### D. Constrained mean-field and deformation

By minimizing the functional, one can only obtains one point of the energy landscape, the ground state. However, one is often interested in the energy surface along specific shape



FIG. 14: (Color online) Illustration of the deviation between the experimental and theoretically computed ground state energy along the nuclear chart. The numbers indicated in the bottom part correspond to the order of magnitude of the energy in this region of mass.



FIG. 15: (Color online) Illustration of the effect of a constraint on the shape of a nucleus. On the left side the nucleus is compressed by adding an external harmonic potential (monopole constraint) while on the right, the nucleus is deformed along one axis (quadrupole contraint)

of nucleus. An example of energy landscape at various compression/dilatation was given in figure 10. Another example of interest to understand the fission of nuclei is the energy it takes as the system becomes more and more elongated along one axis. The simplest way to modify the shape of a system is to add to the single-particle potential a constraint. For instance, to compress the system, it is sufficient to add a harmonic term of the form  $\frac{1}{2}\lambda r^2$ . Then, the system will be more or less compressed depending of the value of  $\lambda$ . Such a term will naturally appear if the minimization is made on  $\mathcal{E}[\rho] - \lambda \langle r^2 \rangle$  instead of  $\mathcal{E}[\rho]$ , this is the so-called Constrained mean-field calculation. More generally, nuclei with various shapes can be obtained by minimizing:

$$\delta(\mathcal{E}[\rho] - \lambda \langle Q \rangle) = 0 \tag{66}$$

 $\lambda$  is then called a Lagrange multiplier while Q is a carefully chosen one-body operator. A schematic illustration of the type of constraint leading to compression or elongation (quadrupole deformation) is shown in figure 15. At the minimum,  $\lambda$  verifies:

$$\lambda = \frac{\partial \mathcal{E}[\rho]}{\partial \langle Q \rangle}.$$
(67)

Typical examples of one-body operators are:

- Monopole: In that case  $Q = Q_{00} = \sum_i r_i^2$ .
- Quadrupole: To form an elongated along the x axis, one can for instance apply the quadrupole constraint with:

$$Q_{20} = \sum_{i} (2\hat{x}_{i}^{2} - \hat{y}_{i}^{2} - \hat{z}_{i}^{2})$$
(68)

• Octupole: octupole deformations corresponds to pear shapes. They could be obtained by applying the operator:

$$Q_{30} = \sum_{i} (\hat{z}_i^3 - \frac{3}{2}\hat{z}_i(\hat{x}_i^2 + \hat{y}_i^2))$$
(69)

• ...



FIG. 16: (Color online) Example of energy landscape obtained from various nuclei as a function of the quadrupole deformation

An illustration of the potential energy landscape obtained for varying quadrupole deformation is shown in figure 16. This figure shows that while in most cases, the minimum of the energy corresponds to spherical nuclei, in some cases, the nucleus is predicted deformed in its ground state. This is indeed confirmed experimentally with for instance the presence of rotational bands in level schemes.

### 1. Some additional remarks on EDF fitting

The infinite nuclear matter properties is not enough to constraint the EDF for finite nuclei. in particular, finite size effects like nuclear surface, shell effects, pairing properties of deformation requires to directly incorporate nuclei properties in the adjustment of the functional parameters. There are currently large efforts to further improve the predicting power of this approach. Below is a list of techniques used to progress in this field:

- Additional constraint on finite nuclei like nuclear binding energy, nuclear radius and/or shell evolution are generally included in the optimization of the functional. The difficulty is to select data that contains new information. Indeed, there exist lots of data on nuclei but not all adds plus value and will be helpful to constraint the functional. The problems, then becomes a tricky information theory problem related to multidimensional fit analysis (see for instance the recent discussion in (Reinhard and Nazarewicz, Phys. Rev. C 81 (2010))).
- One can eventually add new terms based for instance on systematic analysis based on symmetries (see for instance (Carlsson et al, Phys. Rev. C 78 (2008))) or systematic density matrix expansion (Stoitsov et al, Phys. Rev. C 82(2010)). This leads to much more involved functional to be adjusted. For instance, by regarding shell evolution (Otsuka et al, Phys. Rev. Lett. 97 (2006)), the necessity to include a tensor component in the interaction, that has been omitted in EDF in the past, has been pointed out (see Bender et al, Phys. Rev. C 80, (2009) and refs. therein)
- Another way to improve functional approach for nuclei is to break as much as symmetries of the original Hamiltonian as possible (translational invariance, particle number, parity, ...). This aspect will be discussed in more detail below.

#### IV. SYMMETRY BREAKING AND RESTORATION

To describe some many-body correlations in a many-body system, it might be advantageous to use a theory that breaks some symmetries. Let us first clarify what is the meaning of "Symmetry breaking". Let us consider a system described by some hamiltonian  $\hat{H}$ , this Hamiltonian is generally invariant under some transformation. If we denote by  $\hat{G}$  the generator of the considered transformation, such an invariance implies that the Hamiltonian commute with  $\hat{G}$ :

$$[\hat{H}, \hat{G}] = 0.$$
 (70)

If the system evolves, according to the Ehrenfest theorem, we do expect that  $\langle \hat{G} \rangle$  is a conserved quantity. If we are interested in the static properties of the system, due to the commutation of  $\hat{H}$  and  $\hat{G}$ , one can find simultaneously eigenstates of this two operators and the eigenstate can be labelled by the quantum number associated to this symmetry. One can eventually take advantage of the symmetry properties to get solution of a problem. Indeed, by assuming that the many-body wave-function has some symmetries, one can significantly reduce the Hilbert space of wave-function over which a variational principle and find solution that would have been impossible to find otherwise.

It turns out that the opposite is also true. When an approximate solution is searched, like in the Hartree-Fock theory or Energy Density Functional theory, a lower energy can be found if the trial state do not have the proper good quantum number. One see in that case that the symmetry breaking solution can include correlations that would have been impossible to incorporate otherwise. In nuclear physics, one systematically breaks several symmetries. Among the most frequent one, we have translational invariance, rotational invariance, particle number, parity... It should be kept in mind that the symmetry breaking concept is more than a mathematical tool and is deeply connected to the frame we are considering. When we speak about a symmetry of a system, the symmetry is respected in the laboratory frame, while in its *intrinsic frame*, i.e. the frame attached to its center of mass, some symmetries are spontaneously broken. Experimental observation directly points out some spontaneous symmetry breaking (see illustration 17). A system that is translationally invariant, can only have a constant density in space. We have seen that electron scattering probe that nuclei have a finite size with a well localized surface. This is because these experiments probes the density in the intrinsic frame not the lab. frame. Similarly, the existence of rotational bands demonstrate that a nucleus can be deformed, while a system that is rotationally invariant could only be spherical. Again, this stems from the fact that in its intrinsic frame it can be deformed with a definite orientation while in the lab. frame there is no privileged orientation and therefore the wave-function of the system in this frame will be the superposition of all possible orientations and will appear as spherical. As we will see, this average over orientation is at the heart of *Symmetry Restoration*. A more



FIG. 17: Illustration of some symmetries that are often broken in EDF model. In each case, the associated effects that are incorporated by breaking symmetries are shown in the blue box (see text).

abstractive symmetry is the U(1) symmetry associated to particle number conservation. By using quasi-particle states, that are not eigenstates of particle number, one can describe odd-even staggering effect observed in nuclear masses.

## A. An illustrative example: translational invariance

To demystify the concept of symmetry breaking, a simple illustration of translational symmetry breaking is described in this section. Let us consider two interacting particle in one dimension. Assuming an harmonic interaction, the Hamiltonian writes:

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + C(\hat{x}_1 - \hat{x}_2)^2 \tag{71}$$

Since the interaction only depends on the relative distance between particles, the Hamiltonian is automatically translational invariance, i.e.  $[\hat{P}_{\rm cm}, \hat{H}] = 0$ , where  $P_{\rm cm} = \hat{p}_1 + \hat{p}_2$  is the center of mass momentum.

*a.* **Exact solution** An exact solution of the problem can be obtained for this simple problem. Indeed, making the change of variable:

$$\hat{R} = \frac{m_1 \hat{x}_1 + m_2 \hat{x}_2}{m_1 + m_2}, \qquad \hat{r} = \hat{x}_1 - \hat{x}_2,$$
(72)

the Hamiltonian become separable in center of mass and relative distance variables:

$$\hat{H} = \frac{\hat{P}^2}{2M} + \frac{\hat{p}^2}{2\mu} + Cr^2 = \hat{H}_{\text{c.m.}} + \hat{H}_{\text{rel}}.$$
(73)

It is then straightforward to show that the exact wave-function writes as:

$$\Phi(x_1, x_2) = \Psi(R)\phi(r) = \mathcal{N}^{1/2} e^{iP.R/\hbar} e^{-r^2/(2b^2)}$$
(74)

where  $b^2 = \frac{\hbar}{2\mu C}$  with  $\mu = m_1 m_2 / (m_1 + m_2)$ . The energy of the system then writes

$$E_{\text{exact}} = \frac{P^2}{2(m_1 + m_2)} + \sqrt{\frac{\hbar^2 C(m_1 + m_2)}{2m_1 m_2}}$$
(75)

where the first part correspond to the translational energy while the second part is the *intrinsic* energy. From this, one deduce for instance that the probability of the system to be at a given center of mass position is constant:

$$P(R) = \int_{r} dr |\Phi(R, r=0)|^{2} = \frac{1}{\mathcal{N}}$$
(76)

Similarly, the local one-body density  $n(x) = \int_{x_2} |\Phi(x, x_2)|^2 dx_2$  is constant. Indeed, a system that is translationally invariant necessarily has a constant one-body density otherwise a translation of the system would not let it invariant.

b. Symmetry conserving mean-field solution Disregarding the Pauli principle, a mean-field solution can be obtained using a separable wave-packet<sup>8</sup>:

$$\Phi(x_1, x_2) \simeq \varphi_1(x_1)\varphi_2(x_2) \tag{77}$$

The only single-particle states that insure the proper translational symmetry of the state are plane waves, i.e.

$$\varphi_i(x_i) = \frac{1}{L^{1/2}} e^{ip_i x_i}$$
(78)

where for simplicity we assume that the problem is solved in a box of size L. For such a state, the mean-field energy is minimum at  $p_1 = p_2 = 0$ .

<sup>&</sup>lt;sup>8</sup> This can be seen as the Hartree approximation or equivalently, one can assume that single-particle states have spin and that the wave-packet is antisymmetric in spin while the interaction only couple particles with opposite spins

c. Symmetry breaking mean-field solution A solution of the form (Eq. 77) can eventually be obtained by assuming that the Hamiltonian approximate as:

$$\hat{H} \simeq \frac{\hat{p}_1^2}{2m_1} + C\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m_2} + C\hat{x}_2^2 \tag{79}$$

i.e. by neglecting the term  $-2C\hat{x}_1\hat{x}_2$ . This effective Hamiltonian is nothing but the sum of two indendent harmonic oscillators. Its ground state is given by

$$\varphi_i(x_i) = \frac{1}{\sqrt{\pi b_i^2}} e^{-x_i^2/(2b_i^2)}$$
(80)

with  $b_i^2 = \hbar / \sqrt{2m_i C}$  and is associated with an energy:

$$E_{\rm MF} = \varepsilon_1 + \varepsilon_2 = \sqrt{\frac{\hbar^2 C}{2m_1}} + \sqrt{\frac{\hbar^2 C}{2m_2}}$$
(81)

It turns out that such a solution would have been obtained by minimizing the variational principle with unrestricted form of the separable wave-function. This simple example, illustrate many important aspects:

- (i) the minimum of the mean-field energy is reached for a state that is localized in space, therefore it is not an eigenstate of the center of mass. We say in that case that the symmetry is spontaneously broken.
- (ii) By authorizing symmetry breaking, one ends up with an energy that is lower than the one, one could have obtained without breaking it. Or, said differently, the symmetry breaking is a technique to incorporate more correlation than a purely symmetry conserving theory (see illustration in the left side of figure 20). Note that here, what break the symmetry is the state itself.
- (iii) The solution obtained by minimizing the energy written as the expectation of the complete Hamiltonian could equivalently have been obtained using an effective Hamiltonian that do not respect the symmetry (Hamiltonian (79) in the present case)
- (iv) The solution obtained by breaking symmetries is localized in space and can be regarded as a good approximation of the wave-function of the system in its intrinsic frame, the frame attached to its center of mass.
- (v) As an exercise, the model can be further studied by using techniques discussed previously. For instance, constrained Hartree-Fock can be used to impose an average center of mass velocity. This corresponds to minimize

$$\delta\left(\langle\Psi|\hat{H}|\Psi\rangle - E\langle\Psi|\Psi\rangle - v(\langle\Psi|\hat{P}|\Psi\rangle - P)\right) = 0$$
(82)

where P is a real number corresponding to a given center of mass momentum we want to impose. The resulting energy writes:

$$E_{\rm MF} = \frac{P^2}{2M} + \sqrt{\frac{\hbar^2 C}{2m_1}} + \sqrt{\frac{\hbar^2 C}{2m_2}}$$
(83)

This method is a way to account partially for the center of mass kinetic energy contribution. (vi) Note finally, that the part of the Hamiltonian that is neglected in (Hamiltonian (79) will be accounted for if the symmetry is restored (see discussion below).

Below some examples of symmetries that are standardly broken in nuclear physics are discussed.



## B. Deformation

FIG. 18: Illustration of the energy spectra in even nuclei for various deformation. The ratio  $R_{4/2}$  corresponds to the ratio between the difference of energy  $E_{4^+} - E_{0^+}$  and  $E_{2^+} - E_{0^+}$  (courtesy K. Nomura)

In section IIID, we have seen that the constraint Hartree-Fock method can be used in EDF to construct potential energy surfaces as a function of various possible deformation (quadrupole, octupole, ...). Allowing the nucleus to be deformed does not necessarily implies that it is indeed deformed. However, as illustrated in right side of figure 16, the energy of the deformed nucleus can eventually be lower than the energy without deformation. Experimentally, the presence of deformed system in their ground state is clearly signed by the presence of rotational bands in the spectroscopy of nuclei. An illustration of the effect of deformation on nuclear spectra is given in figure 18. The presence of deformation in the ground state of nuclei is rather frequent, the quadrupole deformation generally is dominant while octupole or even tetrahedral deformation are expected to occur much less frequently. In figure 19, an illustration of recent systematic studies of deformation with EDF is shown for the case of quadrupole (left) and octupole (right) deformation

#### C. Pairing correlation in nuclei

The onset of odd-even staggering in nuclei shows that nuclei can gain energy if nucleons can forms pairs. This effect within mean-field is generally accounted for by considering quasiparticle vacuum instead of Slater determinants as a trial state. Such states can eventually



FIG. 19: Illustration of the result of systematic investigation of deformation within EDF. Left: the color indicate nuclei where the ground state is predicted with quadrupole deformation. Right: the black area corresponds to octupole deformation in nuclei ground state.

be written in a BCS form  $as^9$ 

$$|\Phi_0\rangle = \Pi_i (u_i + v_i a_i^{\dagger} a_{\bar{i}}^{\dagger}) |-\rangle \tag{84}$$

where  $\{a_i^{\dagger}, a_i^{\dagger}\}$  corresponds to single-particle states that forms pairs of particles and  $|-\rangle$  is the associated single-particle vacuum. Let us develop above expression as:

$$|\Phi_{0}\rangle = (\Pi_{i}u_{i})|-\rangle + (\Pi_{i\neq j}u_{i})\sum_{j}v_{j}a_{j}^{\dagger}a_{\overline{j}}^{\dagger}|-\rangle + \cdots$$
$$= \sum_{n}c_{n}|\Psi_{n}\rangle$$
(85)

where the first term corresponds to a state with zero particle, the second to a state with two particles (see figure 20)... From this we conclude that such a state is not an eigenstate

<sup>&</sup>lt;sup>9</sup> Here we give an expression that is suitable for even nuclei.



FIG. 20: Illustration of the concept of particle number symmetry breaking when quasi-particle (BCS or HFB) states are used to minimize the energy. Left: the quasi-particle state is not an eigenstate of the particle number operator and can be decomposed onto states with different particle number. Right: Illustration of the use of symmetry breaking state to get energy lower that the one obtained without breaking symmetries. In black, the curve corresponds to the energy landscape obtained without symmetry breaking while the red curve is obtained by breaking symmetries.

of the number of particle operator  $\hat{N} = \sum_{i} a_{i}^{\dagger} a_{i}$ . In terms of symmetry, this corresponds to breaking the U(1) symmetry associated to rotation in gauge space. To insure that the particle number is conserved in average, the variational principle is modified by adding a specific constraint on  $\langle N \rangle$  leading to the minimization:

$$\delta\left(\mathcal{E} - \lambda \langle N \rangle\right) = 0 \tag{86}$$

By using quasi-particle state, one can include correlation beyond the independent particle picture. One way to see it is to realize that the component  $|\Psi_n\rangle$  correspond to a complex mixing of many Slater determinant with particle number n. As discussed in section II B, the use of Slater determinant as trial state insures the optimization of one-body components  $\rho_{ji} = \langle a_i^{\dagger} a_j \rangle$ , when quasi-particle states are used not only  $\rho_{ji}$  components are optimized but also the so-called anomalous density components defined through  $\kappa_{ji} \equiv \langle a_i a_j \rangle$ . An advantage is that now, the correlation matrix defined as:

$$C_{ij,kl} = \rho_{ij;kl}^{(2)} - \rho_{ik}\rho_{jl} - \rho_{il}\rho_{jk}$$
(87)

that is zero for a Slater determinant, reads  $C_{ij,kl} = \kappa_{ij}\kappa_{kl}^*$  and can take non-zero values. The second advantage of quasi-particle state is that most of the theorem that greatly simplify their manipulation (Thouless theorem, Wick theorem, ...) also applies for these states (Ring and Schuck book (1980, Blaizot and Ripka book (1986))).

In the EDF context, the energy becomes a functional of both  $\rho$  and  $\kappa$ . When effective interaction are used to get the functional form, in its simplest form, the functional can be written as:

$$\mathcal{E}[\rho,\kappa] = \sum_{ij} t_{ij} \rho_{ji} + \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl}^{\rho\rho} \rho_{ki} \rho_{lj} + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl}^{\kappa\kappa} \kappa_{ij}^* \kappa_{kl}$$
(88)

where  $\bar{v}^{\rho\rho}$  and  $\bar{v}^{\kappa\kappa}$  stands for the effective interaction used respectively in the mean-field and pairing channels. Note again, that the possibility to use different effective interaction in different channels is due to the flexibility of functional approaches and is at variance with the Hartree-Fock case. A typical form of the interaction used in the pairing channel is :

$$v^{\kappa\kappa} = v_0 \left( 1 - \alpha \left( \frac{\rho}{\rho_0} \right)^{\beta} \right) \delta(r_1 - r_2) \tag{89}$$

where  $\rho_0$  is the saturation density while other parameters are generally adjusted to reproduce the experimental gap  $\Delta$  (see right side of figure 21). In the "standard" terminology,  $\alpha = 0$ corresponds to pure volume interaction and  $\alpha = 1$  to pure surface while other choices correspond to mixed pairing (see left side of figure 21)



FIG. 21: Left: Schematic illustration of the different types of pairing interaction depending on the parameter used in the interaction  $v^{\kappa\kappa}$ . Right: Illustration of the mean experimental gap along the nuclear chart.

#### D. Restoration of broken symmetries and configuration mixing

As discussed above, the possibility to use trial states that explicitly break the symmetry of the underlying many-body Hamiltonian is a powerful tool to incorporate correlation that would have been very difficult to treat otherwise. When comparing with experimental data, we are now facing another dilemma. On one side, it is useful to break as many symmetries as possible, on the other side, true eigenstates of the system are labelled by good quantum numbers. Therefore, a correct description of observation can only be made if symmetries are restored.

To illustrate the essence of symmetry restoration technique let us consider the case of a deformed system. The invariance with respect of rotation (associated to good angular momentum J) imposes that the system is spherical symmetric. As we remark previously, nuclei can really be deformed. This rises the following question: *How can a system be simultaneously deformed and spherical symmetric?* The answer is that the deformation refers to deformation in the *intrinsic frame* attached to the nucleus while the system has good symmetries in the *laboratory frame*. Mean-field calculations are generally made in the intrinsic frame of the nucleus where for instance the axis can be set along the direction of deformation (see figure 22). Let us consider the nucleus in the laboratory frame. In this frame, there is no privileged orientation of the nucleus and any of the orientation leads to the same energy of the system. Said differently all orientation are degenerated. The eigenstate of the system in the lab. frame is obtained from the eigenstates in the intrinsic frame by averaging over all orientations. The average of a deformed system over all orientation will finally leads to a system that is spherical symmetric.

The above discussion is at the heart of the technique used to restore symmetries. One generally introduces the notation of projector onto good quantum number. For instance  $P^{JM}$ ,  $P^N$ , ... denote the projector onto angular momentum J, N, ... Starting with a trial state vector that do not have a good quantum number  $|\Phi(0)\rangle$ , the projector onto quantum number J and M is given by (Ring and Schuck, book (1980)):

$$P_{MK}^J = \frac{2J+1}{8\pi^2} \int_{\Omega} D_{MK}^{J*}(\Omega) R(\Omega) d\Omega$$
(90)

where  $\Omega = (\alpha, \beta, \gamma)$  are the Euler angles,  $R(\Omega) = e^{i\alpha J_z} e^{i\beta J_y} e^{i\gamma J_x}$  is the rotation operator while  $D_{MK}^{J*}(\Omega)$  is the Wigner function that insure the proper weight of each orientation. The rotation operator transform a trial state into another trial state denoted by  $|\Phi(\Omega)\rangle = R(\Omega)|\Phi(0)\rangle$ . Therefore, we see that the state with good quantum number, denoted by  $|\Phi, JM\rangle$  can be written as a mixing of configuration with different orientations:

$$|\Phi, JM\rangle = \int d\Omega f^J_{MK}(\Omega) |\Phi(\Omega)\rangle.$$
(91)

The same type of discussion can be made for other symmetries (see illustration 17). For instance, translational invariance can be restored by averaging over all possible center of mass position (note that in practice this restoration is almost never done exactly and approximate correction to center of mass is used) while projection onto good particle number is made by averaging over the orientations in gauge angle. In the later case, the projector reads:

$$P^{N} = \frac{1}{2\pi} \int_{0}^{2\pi} d\varphi \ e^{i\varphi(\hat{N}-N)} \,.$$
(92)

where  $\varphi$  denotes the gauge angle. Let us consider a state that is a mixing over states with different particle number with  $|\Phi(0)\rangle = \sum_{K} c_{K} |\Psi_{K}\rangle$  as in the case of BCS state. Using the



FIG. 22: Illustration of the different frames (laboratory and intrinsic) used in nuclear physics. The wave-function of a system in the laboratory frame can be obtained by averaging the wave-function of the system in its intrinsic frame over all possible orientations of the intrinsic frame.

fact that:

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi \ e^{i\varphi(K-N)} = \delta(K-N) \tag{93}$$

and that  $\hat{N}|\Psi_K\rangle = K|\Psi_K\rangle$ , we have  $P^N|\Phi(0)\rangle = c_N|\Psi_N\rangle$  and therefore the projection selects only the component with good particle number. Similarly to the rotation case, projection over good particle number can also be interpreted as a mixing over trial state with different gauge angle orientations, i.e. :

$$|\Psi_N\rangle = \int d\varphi f(\varphi) |\Phi(\varphi)\rangle \tag{94}$$

where  $|\Phi(\varphi)\rangle = e^{i\varphi\hat{N}}|\Phi(0)\rangle$ .

Each step, (i) symmetry breaking and (ii) symmetry restoration are expected to further lower the energy. An illustration of the different scales of energy associated to each of the step is given in figure 23. As shown in this figure, the possibility to have symmetry breaking (deformed solution) leads to a gain of more than 10 MeV while the restoration further lower the energy by few MeV. These energy might appear very small compared to the bulk energy ( $\simeq 8.A$  MeV), however this is the level of precision that is required to current EDF theory.



FIG. 23: Illustration of the scale of energy gain due to symmetry breaking and restoration for the case of particle number and deformation symmetry (courtesy M. Bender). In the present example, by authorizing the nucleus to be deformed, one gain 15 MeV, after restoration of the particle number symmetry an extra gain of few MeV is obtained.

#### E. Beyond mean-field: configuration mixing in nuclei

Restoration of broken symmetries provides examples of the configuration mixing technique in nuclei. Configuration mixing can also be used to account for quantum fluctuation associated to some collective variable Q like deformation. Previously, potential energy landscape have been shown where one point of the landscape correspond to a single trial state  $|\Psi(Q)\rangle$ . The description in terms of a single trial state completely neglect the fact that the *true* state might be a mixing of different configuration (deformation). The Generator Coordinate Method (GCM) can be seen as a re-quantization procedure in collective space. Assuming a set of trial state vectors  $\{|\Psi(Q)\rangle\}$ , a new state is defined through:

$$|\Phi\rangle = \int dQ f(Q) |\Psi(Q)\rangle \tag{95}$$

then components f(Q) can be obtained by minimizing the variational principle:

$$\delta\left(\langle \Phi | H | \Phi \rangle - E \langle \Phi | \Phi \rangle\right) = 0 \tag{96}$$

with respect to all variation of the  $f^*(Q)$  while keeping the trial states fixed. This leads to

$$\int dQ' f(Q') \langle \Phi(Q) | H | \Phi(Q') \rangle = E \int dQ' f(Q') \langle \Phi(Q) | \Phi(Q') \rangle$$
(97)

which is nothing but the Hill-Wheeler equation (Ring and Schuck, book (1980)) equivalent to an eigenvalue problem in collective space. It turns out, that the GCM is a powerful tool that not only gives access to improved ground state but can also give excited states.

Ultimately, configuration mixing can be combined with symmetry restoration leading to the trial state:

$$|\Phi:N,JM,...\rangle = \int dQf(Q)P^N P^J_{MK}...|\Psi(Q)\rangle.$$
(98)

This state can be used to minimize the energy leading to the so-called Variation after Projection (VAP) approach to nuclear spectroscopy. Such a calculation is still very challenging today due to (i) the increasing number of degrees of freedom in collective space (ii) the fact that GCM is combined with EDF where basically the off diagonal kernels  $\langle \Phi(Q)|H|\Phi(Q')\rangle$ are not really defined. This has led recently to extensive discussions.



Bender, Duguet, Heenen, Lacroix, Int. J. of Mod. Phys. E (2011) -arXiv:1011.4047

FIG. 24: Left: Schematic illustration of the result of the variational approximation using GCM. The shaded blue area represents the wave-packet component  $|f(Q)|^2$  as a function of the deformation variable Q. Right: Example of results of configuration mixing calculation in mean-field theory leading to the level scheme of <sup>18</sup>O. The different curves corresponds to the different potential energy landscape for specific J values.



FIG. 25: Illustration of the unified description of nuclear structure, dynamics and thermodynamics of nuclei within the EDF(see text).

## V. FINAL REMARKS

In a limited time, it is difficult to cover the full scope of application of mean-field models. The EDF theory is the only framework able at the same time to provide a unified description of nuclear structure, nuclear reactions as well as thermodynamics in nuclei (see illustration 25). In this lecture, due to the allocated short time, I have presented only aspects of mean-field necessary to understand current nuclear structure discussions. Other aspects can be found in many previous interesting lectures given at the Ecole Joliot-Curie. Among them, specific aspects were treated in great details. A non-exhaustive list is given below. In each case, written lectures can be found at the address http://www.cenbg.in2p3.fr/joliot-curie/

- Effective Interaction and associated EDF: (Meyer [1997], ...)
- Symmetry and Symmetry breaking aspects: (Goutte [2010], Schuck [1985]... )
- Collective motion: (Khan [2010], Grasso [2009], Chomaz [1997], ...)
- Large Amplitude dynamics (Simenel [2007], Berger [1991]...)
- Related Nuclear Astrophysics aspects: Grasso [2009], Meyer [1997,2000], Volpe [2000]...

- Non-empirical EDF (Papenbrock [2011], Duguet [2009], Lacroix [2009], Dobaczewski [2002]...)
- ...

### VI. SOME READINGS:

- Quantum Mechanics (vol I and II), A. Messiah, (1958).
- Quantum Mechanics (vol I and II), C. Cohen-Tannoudji, B. Diu, and F. Laloe, (1978).
- Quantum Theory of Many-Particle Systems, A. Fetter and J. D. Walecka, (1971).
- The nuclear Many-Body Problem, P. Ring and P. Schuck, (1980).
- Nuclear Collective Motion: Models and Theory, D. J. Rowe (Re-dedited in 2010).
- Quantum Theory of Finite Systems, J.-P. Blaizot and G. Ripka, (1986).
- Quantum Many-Body Dynamics: application to Nuclear Reactions, C. Simenel, D. Lacroix and B. Avez (2010).
- Basic Ideas and Concepts in Nuclear Physics, K. Heyde (1994).
- The Nuclear Shell Model, K. Heyde (1994)
- Introductory Nuclear Physics, K.S.Krane (1988).
- Physics of the Nucleus, M.A.Preston (1962).
- Nuclear Models, W. Greiner and J.A. Maruhn, (1996).
- Physique des collisions nucléaires, E. Suraud (1998).
- Theory of Nuclear Reactions, P. Fröbrich and R. Lipperheide, (1996).
- Fundamentals of nuclear models, D. J. Rowe and J. L. Wood (2010).
- Density-Functional Theory of Atoms and Molecules, R. G. Parr and W. Yang, (1989).
- Density functional theory: an approach to the quantum many-body problem, R.M. Dreizler and E.K.U. Gross, Springer-Verlag Berlin, (1990).
- A Chemists Guide to Density Functional Theory, W. Koch and M. C. Holthausen, Wiley-VCH, Weinheim, (2001).
- A Primer in Density Functional Theory, C. Fiolhais, F. Nogueira, and M. Marques, volume 620 of Lecture Notes in Physics, Springer, Berlin and Heidelberg, (2003).
- Numerous interesting lectures (in french or english) note given at the International Joliot-Curie School can be downloaded at the address:

http://www.cenbg.in2p3.fr/joliot-curie/