Summary. — The present contribution does not aim at replacing the huge and often excellent literature on DFT for atomic nuclei, but tries to provide an updated introduction to this topic. The goal would be, ideally, to help a fresh M.Sc. or Ph.D. student (or a researcher from other fields) to become acquainted with some basic concepts, and then move to the specialized textbooks or papers with some ability for orienteering. We first introduce the basics of DFT, and show the difference with the “naive” mean-field theory, that is doomed to fail as a model even in the simple case of uniform nuclear matter. We introduce the Energy Density Functionals (EDFs) that are used in nuclear structure, with few examples of their applications. The concepts of symmetry breaking and restoration are briefly discussed. We also include an introduction to the time-dependent extension of DFT that, so far, has been implemented essentially only in the adiabatic approximation and has been applied mainly to the study of nuclear vibrations. With this material, we hope that any reader is able to deal with the texts that go deeper into each of the topics, having understood that DFT is probably the best compromise in nuclear structure theory between simplicity, accuracy, and broad range of applicability.
1. – Introduction

Atomic nuclei are strongly correlated, self-bound quantum systems that are still capturing the interest of so many scientists, more than a century after their discovery, for a variety of reasons.

The nuclear chart, that is a two-dimensional arrangement of nuclei on a plane where the number of neutrons, \( N \), and the number of protons, \( Z \), are the \( x \)- and \( y \)-axis, respectively, has still broad territories to be explored. A schematic view from the web (https://www.nndc.bnl.gov/chart/) is displayed in Fig. 1. Every year, a large number of new nuclei, that amount to \( \approx 20-30 \) in the last decade, are being discovered (cf. [1] and references therein). The limit of existence for neutron-rich or neutron-deficient nuclei (so-called drip lines, beyond which nuclei are unbound with respect to neutron and proton emission, respectively), and the search for superheavy elements, are the highlights of this exploration.

At the same time, the nuclear physics and nuclear astrophysics communities are striving to grasp some understanding of compact objects like neutron stars, that are extreme forms of nuclear matter. While ordinary nuclei display densities around the so-called saturation density \( \rho_0 = 0.16 \text{ fm}^{-3} \) (see below) and are at, or lie close to, zero temperature, different conditions may be realised in stars. The inner core of neutron stars contains...
matter in unknown conditions that may also correspond to a quark-deconfined phase, while the crust is made up with nucleons whose density encompasses a broad range from around $1/3$ to $10^{-3}$ times the saturation density [2]. Neutron stars are believed to contain $\approx 10^{55} - 10^{56}$ neutrons, and as such are displayed in the lower-right corner of Fig. 1.

The new input from nuclei with large neutron-proton asymmetry, or superheavy isotopes, or exotic forms of neutron matter in stars, has changed and is still changing our basic understanding of nuclear structure. Consequently, there is certainly a strong need of up-to-date introductions to several topics.

The present lecture has mainly a theoretical content. Nuclear theory is moving ahead quite rapidly in recent years. Many groups are pursuing the idea that the goal should be deriving nuclear properties from (the low-energy limit of) Quantum Chromo Dynamics (QCD). Genuine lattice calculations with explicit quark degrees of freedom have still serious troubles to reproduce basic properties like the binding energy of the few-nucleon systems (two- and three-body systems turn out to be unbound while $^4$He is severely underbound [3]). A different strategy consists in using an effective realization of the QCD Lagrangian, based on chiral symmetry as originally proposed by S. Weinberg [4]. Chiral Effective Field Theory (EFT) gives rise to a family of model Lagrangians, all based on correct symmetries and separation of energy scales, that can be used in connection with many-body methods like lattice simulations, coupled cluster, renormalization group approaches, or Green’s function methods. These so-called ab initio methods are continuously extending their range of applicability; nonetheless applying them to heavy nuclei, or highly excited states, is still too demanding [5]. More importantly, the quality of the results still depends on the specific Lagrangian [6, 7].

As a summary, deriving nuclear properties directly from QCD is still a long-term project. Ab initio is a wording that may be used in connection with many-body methods that are in principle exact, not only in connection with chiral Lagrangians but also when a phenomenological nucleon-nucleon (NN) interaction is employed. In general, the applicability of these approaches has serious limitations in mass number and excitation energy.

In keeping also with the rich variety of the nuclear phenomena, one can easily understand the absence of a nuclear “standard model”. In the current volume, the reader can browse through different lectures and judge directly about the pros and cons of models like the nuclear Shell Model, the Cluster Model, and the algebraic approaches; all these models necessarily include a fair amount of phenomenological input. DFT lies somehow in between the purely phenomenological models and those that aim at starting from QCD. It can be said in its own way to be an ab initio theory, because it is rooted in the Hohenberg-Kohn theorem (cf. below). There is not, so far, a systematic connection with an underlying theory but many attempts are promising. As we shall argue in this lecture, a reasonable account of experimental data can be achieved in a quite transparent and economic way. Analogies with electronic systems can be traced, having in mind the development of unified methods for many-fermion systems.

The outline of the present contribution is the following. We discuss the basics of DFT, mainly with reference to the electronic systems, in Sec. 2. In the nuclear case, we remind
first the reader about the evidences for independent particle motion that may lead to the assumption of the validity of simple HF (Sec. 3), and we then introduce uniform nuclear matter (Sec. 4) and use it as a playground to show the failure of naïve HF (Sec. 5). We advocate the need for density-dependent interactions that are merely generators of energy functionals, and we discuss the functionals which are currently used in Sec. 6. Few examples of DFT calculations for the ground-state properties are mentioned in Sec. 7. We then move to the concepts of intrinsic density and symmetry breaking in Sec. 8 and Sec. 9, respectively. Sec. 10 is devoted to the extension of DFT to the time-dependent case, with one illustrative example in Sec. 11. Finally, we mention the limitations of DFT in Sec. 12, and we draw some conclusions in Sec. 13.

Many suggestions for further reading are given along the text. Nevertheless, we outline some of them here, for the reader’s convenience. There are standard textbooks that constitute a useful starting point for the study of nuclear structure along the line of this paper [8]. If the reader needs a recent, more introductory text, Ref. [9] is an option. The literature on DFT in condensed matter is huge, and yet we can single out Refs. [10, 11, 12]. Recent, and relatively short, papers on the perspectives for electronic DFT can be found [13, 14]. DFT in nuclear physics has been first reviewed in [15], but the reader can also profit from Refs. [16, 17]. There are many lectures available on the web, and an ambitious and interesting attempt to introduce the subject of DFT in nuclear physics can be found on the archive [18].

Last but not least, we limit ourselves here to a nonrelativistic treatment. Excellent papers that introduce and explain the relativistic (or covariant) nuclear DFT are available [19, 20].

2. – Basics on DFT for electronic systems

We assume we are concerned with a quantum many-fermion system governed by the Hamiltonian

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i \neq j=1}^{N} V(i,j) + \sum_{i=1}^{N} v_{\text{ext}}(i),$$

(1)

where the first term is the kinetic energy of the $N$ fermions having mass $m$, the second term is a two-body interaction in which $i$ is a shorthand notation for the space coordinate, $\vec{r}_i$, spin coordinate and any further degree of freedom (e.g. isospin), and the last term is a possible external potential. In the case of $N$ electrons interacting with the external field of $M$ ions (labelled by $\alpha$, and having charge $Z_\alpha$ and associated coordinate $\vec{R}_\alpha$), this Hamiltonian becomes

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i \neq j=1}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + \sum_{i=1}^{N} \sum_{\alpha=1}^{M} \frac{Z_\alpha e^2}{|\vec{r}_i - \vec{R}_\alpha|},$$

(2)

where the interactions between the ions are not written for the sake of simplicity. The many-body problem associated with this Hamiltonian cannot be solved exactly, even if
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The Coulomb force is well known, and even if one can invoke the Born-Oppenheimer approximation and reduce the whole problem to the electronic problem, for fixed ion positions.

Many strategies have been proposed to solve the many-electron problem. Among them, to the opinion of many, DFT stands out for its conceptual elegance and simplicity (that, most likely, should be a feature of physics as a whole). Its foundation lies in the theorem that bears the name of Hohenberg and Kohn (HK) and that was introduced in their seminal paper [21]. In short, the theorem states that the total energy of the system described by (1), for any external potential \( v_{\text{ext}} \), can be written as a functional of the fermion density \( \rho \) :

\[
E_{v_{\text{ext}}}[^{\rho}] = \langle \Psi | \hat{T} + \hat{V} + \hat{v}_{\text{ext}} | \Psi \rangle = F[^{\rho}] + \int d^3r \, v_{\text{ext}}(\vec{r}) \rho(\vec{r}).
\]

The first equality is just the definition of total energy, while the second equality defines the functional: the contribution of the external potential is singled out and the universal functional \( F \) is introduced. The functional \( E \), Eq. (3), has a minimum at the exact ground-state density where it becomes equal to the exact energy. It is hard to underestimate the value of Eq. (3), because it tells us that the whole information about the ground-state of the system is contained in the one-body density \( \rho \) that is a real function of three coordinates, and we do not need the whole wave function \( \Psi \), that instead is a complex function of \( 3N \) coordinates!

The proof of the theorem can be found in the original paper [21]. We advise the reader to go through it; it is quite instructive, although limited to the specific case in which the ground-state is not degenerate. Extensions of the theorem to the case of degenerate ground states, spin-polarized systems, finite temperature etc.\(^{(1)} \), can be found in the literature (see, e.g., [11]).

The real drawback of the HK theorem is that its proof is merely a proof of existence of the universal functional \( F \). It is not a constructive proof, so that the appropriate strategy to build this functional remains an open problem. A step forward in this direction is represented by the Kohn-Sham (KS) scheme [22], in which it is assumed that the density \( \rho \) can be represented in terms of so-called auxiliary single-particle wave functions (orbitals) \( \phi_j(\vec{r}) \), that is,

\[
\rho(\vec{r}) = \sum_j |\phi_j(\vec{r})|^2.
\]

The index \( j \) labels the orbitals. The meaning of the word “auxiliary” should be clarified here. The orbitals may be looked at as a formal artifact. This does not exclude that, in specific cases, the orbitals turn out to be a fairly good approximation of the actual single-particle wave functions. Within such framework, the total kinetic energy is written

\(^{(1)} \) The list is not exhaustive.
in the usual way,

\[ T = \langle \Psi | \hat{T} | \Psi \rangle = \sum_j \langle j | -\frac{\hbar^2}{2m} \nabla^2 | j \rangle = \sum_j \int d^3 r \phi_j^*(\vec{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \phi_j(\vec{r}), \]  

and the direct Coulomb energy (classical, or Hartree, energy) can be also singled out:

\[ E_{\text{Hartree}} = \frac{e^2}{2} \int d^3 r \ d^3 r' \ \rho(\vec{r}) \rho(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|}. \]  

In this way, the functional (3) is re-written as

\[ E_{\text{KS}} = T + E_{\text{Hartree}} + E_{\text{xc}} + \int d^3 r \ v_{\text{ext}}(\vec{r}) \rho(\vec{r}), \]  

where now the part to be built is the so-called “exchange-correlation” part or \( E_{\text{xc}} \). The minimization of this latter functional with respect to the density should be carried out with the constraint that the orbitals are orthonormal. Therefore, the equations for the orbitals are obtained from

\[ \frac{\delta}{\delta \rho(\vec{r})} \left( E_{\text{KS}} - \epsilon \int d^3 r' \ \phi_j^*(\vec{r}')\phi_j(\vec{r}') \right) = 0, \]  

where the usual symbol \( \delta \) is introduced for the functional derivative. Elementary introductions to functional derivatives can be found in several textbooks (see, e.g., Sec. 3.2 of [23]). Eq. (8), together with Eqs. (7), (5) and (6), leads to the famous Kohn-Sham equations

\[ \left( -\frac{\hbar^2}{2m} \nabla^2 + \frac{e^2}{2} \int d^3 r' \ \rho(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|} + \frac{\delta E_{\text{xc}}}{\delta \rho(\vec{r})} + v_{\text{ext}}(\vec{r}) \right) \phi_j(\vec{r}) = \left( -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{KS}} \right) \phi_j(\vec{r}) = \epsilon \phi_j(\vec{r}), \]  

where we have labelled the total effective Kohn-Sham potential by \( v_{\text{KS}} \), and where the quantities \( \epsilon \) are seen to be the energies associated with the auxiliary orbitals. The reader should note that the total energy is not the sum of these auxiliary energies (this is left as an exercise). We also wish to stress that the variation with respect to \( \rho \) in Eq. (8) has in fact been turned into a variation with respect to the orbitals \( \phi_j^* \).

As for the choice for \( E_{\text{xc}} \), the simplest possible option is to calculate it in a uniform system where translational invariance makes the exact calculation of the total energy feasible. In fact, such a calculation in the limit of high electron densities is analytic and can be found in textbooks (see, e.g., Secs. 3 and 12 of [24] or Sec. 12.3 of [25]). The total energy per particle \( E_N \) reads,

\[ \frac{E}{N} = \frac{e^2}{2a_0} \left( \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622 \ln r_s - 0.094 + \ldots \right) = t + e_x + e_c. \]
One usually defines $a_0 = \frac{\hbar^2}{m e}$ as the Bohr radius, $r_0$ by $\frac{1}{r_0} = \frac{4}{3}\pi r_0^3 m$, so that it is essentially the interparticle spacing, and $r_s = \frac{r_0}{a_0}$. In the latter equation, the dots represent terms of the order $O(r_s \ln r_s)$, and other subleading terms that become negligible at high density, that is, small $r_s$. The first term in brackets in Eq. (10) is the kinetic energy per particle $t$, that goes like $\rho^{2/3}$. In this specific case, the Hartree and external potential contributions cancel exactly\(^{(2)}\). The second term in (10) is the exchange energy $e_x$ while the following terms correspond to the correlation energy $e_c$. For a two-body potential that goes like $1/r$, it is quite intuitive that interaction terms scale at most like the interparticle spacing, or like $\rho^{1/3}$. The different terms of $\frac{E}{N}$ in Eq. (10) are displayed in Fig. 2, where $\frac{E}{N}$ is written as $e$. The total energy has a minimum that mainly results from the balance between the kinetic term that goes like $\rho^{2/3}$ and the exchange term that goes like $\rho^{1/3}$, although the correlation energy plays some role. The minimum corresponds to $r_s$ around 3.8, surprisingly close to the values for real metals that are in the range 3-5. More accurate expressions for the total energy of the uniform electron gas, that are also valid at lower densities, have been derived and are available [26]. Below, we shall compare with the nuclear case.

![Fig. 2. – Energy per particle of the uniform electron gas as a function of the density, within the LDA as discussed in the main text. The curves correspond to the result of Eq. (10) and to the three contributions that appear therein.](image)

\(^{(2)}\) Cf. the discussion in Sec. 3 of Ref. [24].
writes

$$E_{xc} = \int d^3 r \, e_{xc}^{\text{hom}}[\rho(\vec{r})] \rho(\vec{r}),$$

(11)

where we have stressed that the exchange-correlation energy has been taken from the homogeneous gas by means of the superscript. LDA usually produces an overbinding of atoms and molecules, that can be corrected by introducing a dependence of $E_{xc}$ on the gradient of the density, $\nabla \rho$ (Generalized Gradient Approximation, or GGA). At present, increasingly sophisticated functionals that depend also on higher derivatives of the density are discussed and/or start to be built. These various degrees of sophistication are pictorially referred to as a “Jacob’s ladder” [27]. As a last rung of the ladder, a possible dependence on the unoccupied quantum states of the system is postulated. We shall come back to these points when discussing the nuclear case.

3. – The nuclear case: the mean-field picture and Hartree-Fock theory

There are analogies but also important differences between the many-electron problem and the many-nucleon problem. In the latter case there is no external potential, that is, nuclei are self-bound objects. In addition, while in Eq. (1) we have written only a two-body interaction $V(i,j)$, three-body interactions $V(i,j,k)$ are relevant for nuclei and four-body interactions cannot be completely ruled out. As compared with the Coulomb force, the nuclear interaction is short-ranged (the range is of the order of 1 fm), strongly spin-dependent, and characterised by many terms (central, spin, spin-orbit, tensor) of similar importance.

Electron scattering experiments suggest that ordinary nuclei (except the lightest ones) are characterised in their inner part by an approximately constant density, whose value is $\rho_0 \approx 0.16 \text{ fm}^{-3}$ (saturation density) as it has been mentioned in the Introduction. The nuclear surface, although very important for nuclear properties, has a thickness of only $\approx 0.6 \text{ fm}$. As a consequence, the interparticle distance $2r_0$ is $\approx 2.4 \text{ fm}$ and is larger than the range of the nuclear force. In this respect, the nucleus is not a very dense system. Together with the role played by the Pauli exclusion principle, this explains why nucleons do not experience the mutual interaction so often; in fact, it is known experimentally that the nucleon mean free path in nuclei is or the order of, or larger than, the nuclear radius.

Historically, these evidences have led to assuming the validity of mean-field theory, namely of the picture that nucleons move in a one-body potential that results from the average of the interactions with all other nucleons. It has been deemed to be too hard or somehow not so relevant, for many years, trying to deduce the mean-field from a complicated NN Hamiltonian. Empirical potentials like the well-known Woods-Saxon have been often taken for granted. Elegant and sophisticated models have been developed by the Copenhagen school [28, 29], or by Landau and Migdal [30], or by Solovev and co-workers [31], based on single-particle and collective excitations on top of the mean-field, without daring to ask the question whether this mean-field can be derived from an
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underlying theory, or whether binding energies can be calculated therefrom. This lecture deals instead with a unified picture in which the effective mean field can be derived within the DFT framework.

In the 1970s and 1980s, different authors have started to propose effective Hamiltonians with the aim of using them within a microscopic mean-field theory, that is, within Hartree-Fock (HF). One starts from an Hamiltonian analogous to (1),

\[ H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i \neq j=1}^{N} V(i,j), \]

where the difference between the neutron and proton mass has been neglected for the sake of simplicity, and defines an energy functional as

\[ E_{HF}[\rho] = \langle \Phi | H | \Phi \rangle, \]

where \( |\Phi\rangle \) is the most general Slater determinant made up with single-particle wave functions \( \phi_j \). The minimization of this functional, with the same constraint as in Eq. (8), namely

\[ \frac{\delta}{\delta \rho(\vec{r})} \left( E_{HF} - \varepsilon \int d^3r' \phi_j^*(\vec{r}')\phi_j(\vec{r}') \right) = 0, \]

can be carried out in practice replacing the variation with respect to \( \rho \) by the variations with respect to \( \phi_j^* \), and this leads to the well-known HF equations:

\[ \frac{-\hbar^2}{2m} \nabla_j^2 \phi_j(\vec{r}) + \sum_{l=1}^{N} \int d^3r' \phi_l^*(\vec{r}')V(\vec{r},\vec{r}') (\phi_l(\vec{r}')\phi_j(\vec{r}) - \phi_l(\vec{r})\phi_j(\vec{r}')) = \varepsilon_j \phi_j(\vec{r}), \]

where \( P_{12} \) exchanges the particles 1 and 2. The total energy reads

\[ E_{HF} = T + \frac{1}{2} \sum_{jl} \int d^3r \ d^3r' \phi_j^*(\vec{r})\phi_l^*(\vec{r}')V(\vec{r},\vec{r}') (\phi_j(\vec{r})\phi_l(\vec{r}') - \phi_l(\vec{r})\phi_j(\vec{r}')), \]

where \( T \) has the same form as in Eq. (5). We are going now to illustrate that a naïve picture of the nuclear mean-field is doomed to fail, even in the simple case of uniform nuclear matter that is the analogous system with respect to the electron gas that has been previously discussed. In particular, all attempts to account for the empirical evidence(s) using a density-independent effective interaction \( V \), at the HF level, have not been successful.
4. – Uniform nuclear matter

As we have mentioned in the previous Section, the inner part of nuclei displays an approximately constant density, $\rho_0$. In nuclei with $N \approx Z$, proton and neutron densities do not differ too much whereas in nuclei with neutron excess there is a spill-out of the neutron density but not a large difference in the inside part. Thus, we can picture the inside as similar to an extended system having equal number of protons and neutrons and equilibrium density equal to $\rho_0$, that is, similar to a piece of symmetric nuclear matter (SNM). The Bethe-Weizsäcker formula for the energy per particle $e \equiv \frac{E}{A}$, namely

$$e(A, Z) = a_V - a_S A^{-1/3} - a_A \left( \frac{A - 2Z}{A} \right)^2 - a_C Z^2 \frac{A^{1/3}}{A},$$  \hspace{1cm} (17)$$

has an associated volume term $a_V$ of about -16 MeV. If we consider uniform SNM all terms of the mass formula vanish except the volume term. Therefore, it is customary to assume that the energy per particle of this system, at the equilibrium density $\rho_0$, takes the value $e_0 = -16$ MeV. As we have stressed already, this is called the saturation point for SNM.

Around this point, which is a minimum in the energy per particle $e$, one expand this function as

$$e = e_0 + \frac{1}{2} K_\infty \left( \frac{\rho - \rho_0}{3\rho_0} \right)^2 + \ldots,$$  \hspace{1cm} (18)$$

where $K_\infty$ is called nuclear incompressibility, it is proportional to the second derivative $\frac{d^2e}{d\rho^2}$ and, as such, it is related to the stiffness of nuclear matter under compression. Although this quantity can be only indirectly related to observables, like the properties of the compressional-type vibrations of finite nuclei, some bounds on its values have been established in the last decades (see [32] and references therein).

One can also consider the case of asymmetric matter, in which we expect that the energy per particle must depend both on neutron and proton densities $\rho_n$ and $\rho_p$. With a simple change of variables, we can use the total density $\rho$ and the local neutron-proton asymmetry, $\beta \equiv \frac{\rho_n - \rho_p}{2}$. By making a Taylor expansion in $\beta$ and retaining only the quadratic term (odd powers of $\beta$ are obviously forbidden due to isospin symmetry), we can write

$$e(\rho, \beta) = e(\rho, \beta = 0) + S(\rho)\beta^2;$$  \hspace{1cm} (19)$$

where the first term on the r.h.s. is the energy per particle of SNM that we have so far discussed, while the second term defines the so-called symmetry energy $S(\rho)$. From the latter equation, the symmetry energy can be easily understood as the energy per particle that is needed to change symmetric matter into neutron matter.
The symmetry energy can, in turn, be expanded as a function of $\rho$ and, as the saturation point of SNM is a useful reference, one usually writes

$$S(\rho) = J + L \left( \frac{\rho - \rho_0}{3\rho_0} \right) + \frac{1}{2} K_{\text{sym}} \left( \frac{\rho - \rho_0}{3\rho_0} \right)^2 + \ldots,$$

where $J$ is the value of the symmetry energy at saturation density and the other parameters are related to the first and second derivatives at the same point. In particular, $L$ is often referred to as the “slope parameter”. Constraints on the values of $J$ and $L$ have been established by the study of phenomena in which a neutron-proton imbalance is created at different densities, like oscillations where protons and neutrons vibrate out of phase or heavy-ion collisions where projectile and target have different composition; masses as a function of the neutron excess, or observations of neutron stars, can also help in constraining the values of $J$ and $L$ (cf. Refs. [33, 34, 35, 36, 37]).

5. – Failure of mean-field with simple forces and the need for DFT

In SNM the Fermi momentum is given by

$$k_F = \left( \frac{3\pi^2 \rho}{2} \right)^{1/3},$$

and, at saturation density, it takes the value $\approx 1.33$ fm$^{-1}$. The wave functions in a uniform system are plane waves due to translational invariance. This simplifies the calculation of the total energy (16), in keeping with the well-known replacements

$$\phi_j(\vec{r}) \rightarrow \frac{1}{\sqrt{\Omega}} e^{i\vec{k} \cdot \vec{r}}$$

$$\sum_j \rightarrow \frac{g\Omega}{(2\pi)^3} \int d^3k,$$

where $g = 4$ is the degeneracy and $\Omega$ is the quantisation volume. The kinetic part $T$ of the total energy can be calculated straightforwardly and re-expressed in terms of the density thanks to Eq. (21). The kinetic energy per particle, $t$, is

$$t = \frac{T}{A} = \frac{2}{\pi^2} \frac{\hbar^2 k_F^2 \Omega}{2m} \frac{3}{5} \left( \frac{3\pi^2}{2} \right)^{2/3} \frac{\hbar^2}{2m} \frac{2^{2/3}}{\rho^{2/3}}.$$

Now, the question arises under which conditions, within simple HF, an effective force $V$ allows nuclear saturation. In terms of radial dependence, Yukawa functions may

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$^{(3)}$ The presence of two neutrons and two protons for each value of the momentum $\vec{k}$, namely the degeneracy $g = 4$, makes the factor in the next equation different from that of the electronic case.
constitute a choice as they resemble what is deduced from the Fourier transform of a massive boson propagator. Gaussian functions have also been, and still are, used because they allow an easy calculation of the matrix elements on a harmonic oscillator basis [38]. From the viewpoint of EFT, if one is interested in nuclear properties at the scale of tens of MeV or less, the details of the radial shape of the force on a scale around 1 fm should be unimportant\(^4\). Intuitively, nuclear saturation should emerge from a balance between some attractive and repulsive mechanisms and we will discuss briefly the minimal number of terms that have to be introduced to this aim, sticking to a nonrelativistic picture as already mentioned\(^5\).

For a single Gaussian interaction having a range \(\mu\),

\[
V(\vec{r}_1, \vec{r}_2) = Se^{-\frac{|\vec{r}_1 - \vec{r}_2|^2}{\mu^2}},
\]

the direct and exchange terms of the total energy per particle, \(v_H\) and \(v_x\), calculated from Eq. (16), read\(^6\)

\[
v_H = \frac{S}{2} \frac{\mu^3 \pi^{3/2}}{\rho},
\]

\[
v_x = -\frac{S}{2} \frac{1}{\sqrt{\pi}} g(\mu k_F),
\]

where \(g(x) = \frac{2}{\sqrt{\pi}} - \frac{3}{2} - \left(\frac{2}{\sqrt{\pi}} - \frac{1}{2}\right) e^{-x^2} + \sqrt{\pi} \text{erf}(x)\) [40, 41]. One can immediately notice that the direct term goes like \(\rho\), as it must be for a short-range two-body interaction, and in contrast with the case of the electron gas. The exchange term has opposite sign, and a more subtle density dependence that can nevertheless be easily inferred. The force is attractive \((S < 0)\), and it turns out by inspection that the repulsion from the exchange term plus the kinetic energy is far too weak to allow saturation. A possible way out, as already suggested long ago by Brink and Boeker [42], is to introduce exchange terms in the interaction. For instance, Eq. (24) can be generalised to

\[
V(\vec{r}_1, \vec{r}_2) = S(1 - m + mP_M)e^{-\frac{|\vec{r}_1 - \vec{r}_2|^2}{\mu^2}},
\]

where \(P_M\) is the operator that exchanges the particles 1 and 2. Then, the potential

\(^4\) The reader should remember that \(\hbar c = 197.3\) MeV fm, and this allows making the equivalence between 1 fm and about 200 MeV. Natural units embed such concepts but will not be used throughout this lecture.

\(^5\) The mechanism for saturation in a covariant theory (balance between scalar and vector potentials) is discussed in the original paper by Serot and Walecka [39], as well as in the aforementioned references [16, 19].

\(^6\) The calculation is straightforward, although some integrals are not elementary as discussed in the Coulomb case in Ref. [24].
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energies per particle of Eq. (25) become

\[ v_H = \frac{S}{8} (4 - 5m) \mu^3 \pi^{3/2} \rho, \]
\[ v_x = \frac{S}{2} (5m - 1) \frac{1}{\sqrt{\pi}} g(\mu k_F). \]

In this way, the weight of the different terms is changed, and saturation becomes possible for values of \( \mu \) that lie approximately in the range \( 0.5 \, \text{fm} < \mu < 1.5 \, \text{fm} \) [42]. An example of calculation of the HF energy per particle, performed with a force of this type [41], is shown in Fig. 3 and compared with the result of a Skyrme functional that is discussed in the next Section. Similar arguments apply in the case of a Yukawa interaction: only exchange terms allow saturation, as it was remarked in Sec. 2.3.1 of [43] where one can also find the formulas that are analogous to Eq. (27) (cf. also [44]).

\[ \rho \]
\[ 0.05 \, \text{fm}^{-3} \]
\[ 0.1 \]
\[ 0.15 \]
\[ 0.2 \]
\[ 0.25 \]
\[ 0.3 \]
\[ 0.35 \]
\[ 0.4 \]
\[ 0.45 \]
\[ 0.5 \]
\[ e[\text{MeV}] \]
\[ 15 \]
\[ 10 \]
\[ 5 \]
\[ 0 \]
\[ -5 \]
\[ -10 \]
\[ -15 \]
\[ 0 \]
\[ 0.05 \]
\[ 0.1 \]
\[ 0.15 \]
\[ 0.2 \]
\[ 0.25 \]
\[ 0.3 \]
\[ 0.35 \]
\[ 0.4 \]
\[ 0.45 \]
\[ 0.5 \]

Fig. 3 – Energy per particle in symmetric nuclear matter, calculated either with a force of the type (26) and parameters \( S = -429.83 \, \text{MeV}, \, m = 1.3218, \, \mu = 0.8343 \, \text{fm} \) (blue curve), or with a simplified Skyrme functional of the type (34) and parameters \( t_0 = -2552.84 \, \text{MeV-fm}^3, \, t_3 = 16694.7 \, \text{MeV-fm}^{3(\alpha+1)}, \, \alpha = 0.20309 \).

The simple forces that we have described earlier in this Section do not possess necessarily enough flexibility to reproduce the empirical values of \( K_\infty, \, J \) and \( L \). Certainly, one could complicate them and introduce more Gaussian (or Yukawa) terms with different ranges, different exchange operators etc. What seems, so far, impossible to obtain in such naïve mean-field scheme is the empirical value of the effective mass, \( m^*/m \).

In a uniform system, the most general way to write the single-particle dispersion relation, namely the relation between energy and momentum (which is the only available
quantum number), reads

\[ \varepsilon = \frac{\hbar^2 k^2}{2m} + \Sigma(k, \varepsilon) \equiv \frac{\hbar^2 k^2}{2m^*}, \]

where \( \Sigma \) is the single-particle self-energy. The second equality is the definition of the effective mass, and by further elementary steps [45] one can arrive at

\[ m^* = m \left( 1 + m \frac{\partial \Sigma}{\hbar^2 k \partial k} \right) \left( 1 - \frac{\partial \Sigma}{\partial \varepsilon} \right)^{-1}. \]

The HF equations of the second line in Eq. (15), in the case in which the wave function is a plane wave as in (22), can be easily cast in the form (28). In a simple way, one obtains

\[ \Sigma_{\sigma\tau}(k, \varepsilon) = \sum_{\sigma', \tau'} \frac{\Omega}{(2\pi)^3} \int d^3k' \langle \vec{k}, \sigma, \tau; \vec{k}', \sigma', \tau' | V (1 - P_{12}) | \vec{k}, \sigma, \tau; \vec{k}', \sigma', \tau' \rangle, \]

where we have explicitly introduced the sum over the spin and isospin degrees of freedom (\( \tau \) labels either neutrons or protons). We expect that \( \Sigma \) depends on \( \sigma \) (\( \tau \)) only in the case of polarized (neutron-proton asymmetric) matter. Once \( V \) is given, \( \Sigma \) can be calculated and the effective mass can be extracted therefrom. One can explicitly see that, within HF, \( \Sigma \) does not depend on \( \varepsilon \). The non-trivial value of \( m^*/m \) is brought by the \( k \)-dependence of \( \Sigma \) that comes from exchange terms.

From its definition (28), the effective mass is clearly related to the level density: the larger its value, the smaller the level spacing. In a non-uniform system the picture is less simple, but nevertheless the whole nuclear phenomenology is consistent with a value of the effective mass \( m^*/m \) lying in the range \( \approx 0.7-1.0 \). This has been established for quite a long time (cf. the very comprehensive review paper [45], where also the density and energy dependence of the effective mass is addressed). The simple HF that we have described so far, leads to much smaller values (between 0.2 and 0.4). This problem is discussed in detail in Refs. [46, 47, 48] (cf. also [41, 44, 49]).

So far, it has not been possible to design an effective \( V \) that provides a successful description both of the bulk nuclear properties (nuclear saturation and properties of uniform matter around \( \rho_0 \), as well as masses and radii of finite nuclei as we discuss below) and of nuclear spectroscopic properties (effective mass, viz. level density), without introducing a density dependence in the Hamiltonian.

A density-dependent \( V[\rho] \) or \( H[\rho] \) has, generally speaking, conceptual problems unless one considers it merely as a way to generate an energy functional through Eq. (13), that is,

\[ E[\rho] = \langle \Phi | H[\rho] | \Phi \rangle. \]
In this respect, we can conclude that DFT, and not HF, is a viable theory for nuclei in our current understanding. A similar argument can be found under different forms in the literature [47].

6. – Examples of nuclear EDFs

The finite-range Gogny force [50, 51] is the generalisation of the Brink-Boeker force that we have introduced in the previous Section. It reads:

$$V_{\text{Gogny}}(\vec{r}_1, \vec{r}_2) = \sum_{j=1}^{2} e^{-\mu_j |\vec{r}_1 - \vec{r}_2|^2} \left( W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau \right) + t_3 \left( 1 + x_0 P_\sigma \right) \delta(\vec{r}_1 - \vec{r}_2) \rho^\sigma \left( \frac{\vec{r}_1 + \vec{r}_2}{2} \right) + i W_{ls} (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k} \times \delta(\vec{r}_1 - \vec{r}_2) \vec{k},$$

(32)

where $P_\sigma = \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$ is the spin-exchange operator, $P_\tau = \frac{1}{2}(1 + \vec{\tau}_1 \cdot \vec{\tau}_2)$ is the isospin-exchange operator, $\vec{k} = -\frac{i}{2} \left( \vec{\nabla}_1 - \vec{\nabla}_2 \right)$ is the relative momentum operator acting at right and $\vec{k}^\dagger$ is the adjoint operator acting at left. The interaction is the sum of two Gaussians with exchange operators, a density-dependent term and a spin-orbit term. The density dependent term has been deemed to be essential to obtain a reasonable single-particle level density (cf. our discussion of the effective mass in the last Section). This term must be zero-range to avoid ambiguities on the point where the density must be evaluated. The spin-orbit term is also zero-range, for simplicity. This interaction has 14 free parameters to be adjusted.

Another class of successful effective interactions is based on the zero-range, momentum-dependent Skyrme ansatz [52, 53, 54]:

$$V_{\text{Skyrme}}(\vec{r}_1, \vec{r}_2) = t_0 \left( 1 + x_0 P_\sigma \right) \delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{2} t_1 \left( 1 + x_1 P_\sigma \right) \left( \vec{k}^2 \delta(\vec{r}_1 - \vec{r}_2) + \delta(\vec{r}_1 - \vec{r}_2) \vec{k}^2 \right) + t_2 \left( 1 + x_2 P_\sigma \right) \vec{k}^\dagger \cdot \delta(\vec{r}_1 - \vec{r}_2) \vec{k} + \frac{1}{6} t_3 \left( 1 + x_3 P_\sigma \right) \delta(\vec{r}_1 - \vec{r}_2) \rho^\sigma \left( \frac{\vec{r}_1 + \vec{r}_2}{2} \right) + i W_0 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}^\dagger \times \delta(\vec{r}_1 - \vec{r}_2) \vec{k},$$

(33)

where now there are 10 free parameters to be adjusted. As we have just mentioned, a density-dependent force is just a way to generate an energy functional through Eq. (31). It is a good exercise for the reader to show that a simplified Skyrme force without momentum and spin dependence,

$$V(\vec{r}_1, \vec{r}_2) = t_0 \delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{6} t_3 \left( 1 + x_3 P_\sigma \right) \delta(\vec{r}_1 - \vec{r}_2) \rho^\sigma \left( \frac{\vec{r}_1 + \vec{r}_2}{2} \right),$$

(34)

generates for even-even systems the functional

$$E[\rho_n, \rho_p] = \int d^3r \ E[\rho_n, \rho_p].$$
\[ E[\rho_n, \rho_p] = \frac{\hbar^2}{2m} \tau + \frac{1}{2} t_0 \left( \rho^2 - \frac{1}{2} \left( \rho_n^2 + \rho_p^2 \right) \right) + \frac{1}{12} t_3 \left( \rho^{\alpha+2} - \frac{1}{2} \rho^\alpha \left( \rho_n^2 + \rho_p^2 \right) \right). \]  

In these latter equations, the total energy \( E \) is written in terms of the energy density \( E \). Thus, one speaks (in this and all cases to be discussed below) of \( E \) as of an energy density functional (EDF), namely an energy density that depends on functions like \( \rho_n \) and \( \rho_p \). Zero-range forces generate local functionals (at variance with the Coulomb case that has been previously discussed). Fractional power dependences like \( \rho^\alpha \) cannot come from density-independent two-body, three-body, or many-body forces. In other terms, they mimic many-body effects in a more subtle way. It has been known for many years now that only functionals in which such fractional powers appear, reproduce the empirical values of \( K_\infty \) [43, 32]. The kinetic part of the Hamiltonian introduces the first term appearing in the r.h.s. of Eq. (35), that depends on the so-called kinetic energy density,

\[ \tau = \sum_j |\nabla \phi_j|^2. \]  

The whole Skyrme force (33) includes momentum-dependent terms that bring a dependence on \( \tau \) into the potential energy density as well, together with a dependence on \( \nabla \rho \).

The complete EDF associated with a Skyrme force can be found, for even-even systems, in Refs. [53, 54]. More densities appear like the spin-orbit densities \( \vec{J} (\vec{r}) \). Interestingly, terms that depend on the same kinds of densities that have been introduced for electron systems in [27], characterise the Skyrme EDFs. A finite-range force like the Gogny interaction produces a non-local EDF.

In fact, the very idea that an Hamiltonian including a density-dependent force is the tool to generate an EDF has been abandoned by most groups. A functional can be directly parameterized in terms of local densities, without any reference to an underlying interaction. A pioneering step in this direction was taken by Reinhard and Flocard [55] more than twenty years ago, as they wrote the spin-orbit part of their EDFs without reference to a specific form of the force. Later, this has become the customary procedure, e.g. for functionals of the UNEDF family [56].

All possible local densities that can appear in an EDF, have been classified in Refs. [57, 58, 59, 15] (see also [60]). The nuclear EDF must be invariant with respect to parity, time-reversal, rotational, translational and isospin transformations (details can be found in the quoted works). Time-reversal plays a special role here. Densities can be either time-even or time-odd but the latter vanish in even-even systems. Thus, the EDF can be made up with terms that are bilinear in either types of densities, but the terms that are bilinear in time-odd densities do not vanish only in systems with an odd number of particles. A current open questions for practitioners and not only, is to which extent higher and higher gradients of the density are needed for an EDF in order to satisfactorily account for nuclear properties [61, 62, 63].

This discussion is of course not exhaustive. Other forces have been considered as generators of EDFs, for examples semi-realistic forces of Yukawa type with density-dependent terms [64]. Other kinds of functionals have been proposed by Fayans and
collaborators [65, 66]. We do not discuss all the attempts to derive functionals from underlying theories like Brückner-Hartree-Fock [67] or chiral forces.

7. – Examples of calculations of ground-state properties

The main observable that one aims at calculating with an EDF, is the total energy which is actually the binding energy of a nucleus and can be compared with very accurate experimental data. The typical errors are of the order of \(\approx 1-2\) MeV. While this accuracy may be thought to be small, at least in comparison with total binding energies that span values like \(10^2-10^3\) MeV, one should keep in mind that nuclear processes like reactions and decays depend on differences of binding energies, that may be small. This is the motivation for reducing these errors with respect to experiment. Models that include macroscopic ingredients in alternative, or in addition, to the pure implementation of DFT may reach accuracies of the order of hundreds of keV (cf. the review paper [68] or, for more recent advances, [69] and references therein).

In Fig. 4 we show examples of comparison between experimental binding energies and the result of DFT calculations. The Skyrme functional SLy4 [54] has been fitted by using masses and charge radii of basically only magic nuclei. This is probably the reason of the archlike behaviour, which is common to many EDFs. Reproducing with similar accuracy closed-shell and open-shell nuclei still represents a challenge. More modern functionals like UNEDF0 [70] seem to behave much better than SLy4, although the trend of the
error as a function of the neutron number is not really flat. The reader should be also aware of the significant recent progress in DFT calculations using covariant functionals, not discussed in this contribution: a careful analysis of the mass residuals, and their link(s) with other features of the EDFs, is carried out in Ref. [71]. To which extent some correlations that are relevant for nuclear masses cannot be captured by DFT calculations, is still an open question.

EDFs have been applied to predict the limits of nuclear stability, namely the position of the drip lines that we have mentioned in the Introduction [72, 73]. Other relevant ground-state observables are radii and density distributions. Charge radii are available for comparison with experiment: EDFs may display errors of the order of 0.02-0.03 fm, typically. As far as isotopic trends of radii are concerned, while in many instances EDFs perform well, there are still specific unresolved issues (cf. Fig. 11 of [15]: the isotopic dependence of the charge radii along the Ca chain is a typical case where EDFs fail). Last but not least, there is strong current interest in measuring neutron radii or density distributions; EDFs provide predictions than span a relatively broad interval for neutron radii, and fixing this observable would be of paramount importance for our understanding of the nuclear symmetry energy (see the discussion in Sec. 4, and the references therein).

8. – Intrinsic density

The biggest difference between DFT in finite electronic systems and nuclei consists in the fact that in the former case, in most instances, the fixed ion positions constrain the shape of the system in the laboratory frame. In nuclei, that are self-bound systems, this is not the case. The usual HK theorem, as it has been argued by several authors [74], is irrelevant to the nuclear case because it concerns the laboratory density, while experiments probe the intrinsic density (relative to the nuclear center of mass).

 Nonetheless, it has been proven that, at least in principle, given an arbitrary Hermitian operator $\hat{Q}$, one can build an energy functional depending on $Q(\vec{r}) \equiv \langle \hat{Q}(\vec{r}) \rangle$ that is universal in the HK sense and has its minimum at the correct value of $Q$ with the correct energy. In this respect, one can replace the laboratory density with the intrinsic density in the HK theorem [74, 75, 76].

A very interesting point is that the intrinsic density appears to break, in many cases, the symmetries associated with the Hamiltonian as we discuss in the next Section.

9. – Symmetry breaking and restoration

In general, if the Hamiltonian of a system commutes with a given symmetry operator $S$,

$$[H, S] = 0,$$

one expects to be able to find eigenstates of the system which are also eigenstates of $S$. The problem with this statement of principle comes when one is forced to treat
strongly correlated systems and to resort to approximations. In that case, a symmetry-conserving solution may be much less realistic, within the approximated framework, than a symmetry-breaking one.

The first example is that of translational symmetry. A very simple example borrowed from [77, 78] will highlight the above statements. Let us consider two particles in 1D, confined in the interval $-L/2 < x < L/2$, interacting through an harmonic potential,

$$
H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{C}{L^2} (x_1 - x_2)^2.
$$

(38)

By using the center-of-mass and relative coordinates $R = \frac{x_1 + x_2}{2}$ and $r = x_1 - x_2$, together with the associated momenta $P$ and $p$, respectively, this Hamiltonian can be separated into center-of-mass and intrinsic Hamiltonians,

$$
H = \frac{P^2}{4m} + \frac{p^2}{m} + \frac{C}{L^2} r^2 = H_{\text{COM}} + H_{\text{intr}}.
$$

(39)

This Hamiltonian clearly commutes with the total momentum $P$, that is, it manifests the translational invariance. The exact wave function is known, namely it is a product of a free particle times a harmonic oscillator wave function, it is an eigenstate of $P$, and the associated energy is

$$
E_{\text{exact}} = \frac{P^2}{4m} + \sqrt{\frac{\hbar^2 C}{mL^2}}.
$$

(40)

Let us now imagine that we restrict ourselves to products of independent wave functions. If the two particles are bosons, or spin 1/2 fermions in a spin-antisymmetric state(7), the total wave function is

$$
\Phi = \phi_1(x_1) \phi_2(x_2).
$$

(41)

Imposing translational invariance here, would amount to take the $\phi$ as plane waves which means $\phi_i(x_i) = \frac{\exp(ip_i x_i / \hbar)}{\sqrt{L}}$. The expectation value,

$$
E = \langle \Phi | H | \Phi \rangle,
$$

(42)

can be easily calculated by using the Hamiltonian in the form (38), and one can verify that its value is significantly different from the exact one of (40). If we use the independent particle ansatz (41) and we give up the requirement of translational invariance, the

---

(7) We would like to avoid antisimmetrization in order to simplify the pedagogical argument we are developing.
minimization of (42) produces instead an intrinsic energy given by

\[ E_{\text{symm. breaking}} = 2\sqrt{\frac{\hbar^2 C}{2mL^2}}, \]  

with an associated wave function that is the product of two localized harmonic oscillators. This energy is relatively close to the intrinsic part of the exact one, that is, the second term at the r.h.s. of Eq. (40).

The above example should make clear why the choice of using the variational ansatz with symmetry-breaking wave functions might be preferable to other options. Translational symmetry and its breaking characterizes all systems, and it is not of special relevance for the atomic nucleus. On the other hand, rotation and gauge symmetries, that we shall now discuss, are instead associated with the quadrupole and pairing correlations that have been identified as the most important correlations in finite nuclei since several decades.

To make the introduction to rotational symmetry and its breaking as simple as possible, let us pick up another very simple example, by considering several particles in a 3D harmonic one-body potential plus a zero-range two-body residual interaction. The corresponding Hamiltonian reads

\[ H = \sum_i \frac{\vec{p}_i^2}{2m} + \sum_i \frac{1}{2}m\omega^2 r_i^2 + \frac{1}{2} \sum_{ij} \epsilon \delta(\vec{r}_i - \vec{r}_j), \]

where \( \epsilon \) is small so that the residual interaction term will be treated as a perturbation of the 3D harmonic oscillator. The particles in this potential have eigenstates \( |nlm\rangle \), with associated energies \( E_{nl} = \hbar \omega \left( 2n + l - \frac{1}{2} \right) \) and wave functions \( \phi_{nlm}(\vec{r}) = u_{nl}(r) Y_{lm}(\theta, \phi) \), where the radial part can be explicitly written in terms of Laguerre polynomials. If these particles are fermions, they occupy the states 1s, 1p etc.

If we have a set of orbitals that are filled and we add one particle, this will occupy the lowest unoccupied orbital. The perturbing zero-range interaction [last term in Eq. (44)] has been assumed to be weak and, consequently, unable to alter the structure of the orbitals and shells. Nevertheless, if we add a second particle this will produce at lowest order an energy shift \( \Delta E \) given by

\[ \Delta E = \epsilon \langle nlm, nlm' | \delta(\vec{r}_1 - \vec{r}_2) | nlm, nlm' \rangle, \]

where \( m, m' \) are the quantum numbers of the two particles in the degenerate levels. This
Density Functional Theory (DFT) for atomic nuclei: a simple introduction

Table I. – Values of \( f(m, m') \) defined in the main text.

| \( m/m' \) | -2 | -1 | 0  | 1  | 2  |
|-----------|----|----|----|----|----|
| -2        |    |    | 0.227 |    |    | 0.455 |
| -1        | 0.227 |    | 0.227 | 0.455 |    | 0.227 |
| 0         | 0.227 | 0.227 |    | 0.227 |    |    |
| 1         | 0.227 | 0.455 | 0.227 |    |    | 0.227 |
| 2         | 0.455 | 0.227 | 0.227 | 0.227 |    |    |

The shift can be calculated and the result reads

\[
\Delta E = \epsilon \int dr \frac{u_{nl}(r)}{r^2} \sum_{\lambda} \frac{2\lambda + 1}{4\pi} \langle l m \lambda 0 | l m \rangle \langle l m' \lambda 0 | l m' \rangle \langle 0 \lambda 0 | 0 \rangle^2,
\]

where the sum is limited by the angular momentum selection rules, that are implicit in the Clebsch-Gordan coefficients.

The values of \( f(m, m') = \frac{\Delta E}{\epsilon \int dr u_{nl}(r)r^{-2}} \) are displayed in Table I for the case of \( l = 2 \) (d orbitals). The diagonal values are excluded from the Table because the two particles cannot occupy the same quantum states. The largest values are those with \( m' = -m \). This can be intuitively understood in a qualitative way, since the two orbitals with the same absolute value of \( m \) have the largest spatial overlap so that a short-range interaction has the largest effect. If such short-range interaction is attractive, two particles will let the system gain energy if the orbitals with \( |m| = 2 \) are occupied, that is, the system has a non-spherical shape. This deformation is enhanced by polarization effects, namely by the interaction between the particles in the last orbitals and the others. The details of polarization effects go beyond the scope of this lecture. Nevertheless, these effects contribute to make the nucleus deformed as a whole.

Quadrupole deformations are, by far, those dominant along the nuclear chart. Nuclei with quadrupole deformation have been identified by their rotational bands, that is, in keeping with the fact that their spectra correspond to those of a rotor [29]. Also, octupole correlations and octupole deformations have been subject of recent interest and have been now unambiguously proven [79, 80].

If the quadrupole deformed configuration of the system corresponds to a deep minimum of the total energy, that is, the total energy has a stiff behaviour around this minimum, DFT describes well, as a rule, the rotational spectra or at least the lowest sector of the rotational bands [15]. Phenomena that take place when the rotation is fast as the angular momentum is large, or hyperdeformation, are discussed in the literature and also dealt with in the nuclear DFT context (see e.g. Ref. [58]).

(8) The multipole expansion of the delta function, and the matrix elements of the spherical harmonics, are needed.
As is clear from the previous discussion, deformation occurs in the center-of-mass frame. Thus, we have spontaneous symmetry breaking in the intrinsic system. The way in which the symmetry is restored is by means of rotation in the laboratory system, that is, by superimposing different shapes that are produced through a rotation by a set of Euler angles $\Omega$. This is depicted schematically, in 2D, in Fig. 5. Since the result of the rotation of a spherical harmonic $Y_{lm}$ by $\Omega$ is given by $\sum_{m'} D_{lm}^{l'} (\Omega) Y_{l'm'}$, where $D$ is a Wigner function, the wave function associated with the superposition of states $l, m'$ that are rotated reads

$$|nlm\rangle = N \int d\Omega \ D_{l'm'n}(\Omega)|nlm'\rangle,$$

where $N$ is a normalization factor. This can be also interpreted as a projection on good angular momentum in the laboratory frame. Superimposing different shapes, and restoring the rotational symmetry by means of this angular momentum projection, is called multi-reference DFT (MR-DFT) in the context of nuclear EDFs. There is rapid development in recent years concerning MR-DFT, using the Skyrme and Gogny functionals that have been discussed in Sec. 6 as well as using the covariant functionals.

A similar, yet more abstract, reasoning holds in the case of the pairing correlations \cite{81}. Open-shell nuclei are characterised by the fact that a fraction of nucleons around the Fermi energy display a superfluid character. Their phenomenology is, as a rule, well described by the BCS (Bardeen-Cooper-Schrieffer) theory. Within this framework, nucleons in time-reversal states form so-called Cooper pairs, and the superfluidity is associated with the coherent behaviour of these fermion pairs that are quasi-bosons. A very economic way to introduce pairs that are made up with fermions in time-reversal states is the BCS ansatz for the many-body wave function, that reads

$$|\Phi\rangle = \Pi_j \left( u_j + v_j a_j^\dagger a_j^\dagger \right) |-\rangle,$$

where $j$ labels a set of single-particle orbitals like the $\phi_j$ that have been previously
discussed, \( a_j \) and \( a_j^\dagger \) are, respectively, the annihilation and creation operators that destroy or add a particle in these orbitals, and the symbol \( j \) indicates the time-reversal operation on \( j \).

This wave function is clearly a superposition of components with different number of particles. Within the BCS theory, one determines the orbitals \( \phi_j \), the parameters \( u_j \) and \( v_j \) that appear in (48), and other relevant quantities, by minimisation of the total energy (see Ch. 6 of Ref. [8]). The most relevant quantity is the pairing gap \( \Delta \), that corresponds to the minimal excitation energy of the system and can be interpreted as the binding energy of the Cooper pairs. The results of BCS can be compared with the experimental findings, and the success of the comparison is, in the present context, a further example of a symmetry-breaking wave function that describes nuclei more efficiently than a symmetry-conserving one. The symmetry restoration can be realised in a similar way as in Eq. (47), through a rotation in an abstract space by the so-called gauge angle. The reader is advised to consult Refs. [8, 81]. The generalisation of BCS, namely the Hartree-Fock-Bogoliubov (HFB) theory, is also described in [8]. Nowadays, the evolution of pairing when going towards the drip lines, or in other dilute systems like the crust of neutron stars, is under discussion. Another subject which is of great interest, but goes beyond the scope of this lecture, is whether pairing between protons and neutron is strong enough to give rise to a condensate [82].

In summary, space deformation and pairing are both characterised by non-vanishing expectation values of operators that correspond to the broken symmetries in the intrinsic system. In the case of quadrupole deformation, the expectation value of the quadrupole moment \( \hat{Q} \) shows up. One can of course generalise to other deformations like octupole. In the case of pairing, where the wave function (48) mixes states that differ by two particles, the non-vanishing expectation value is that of \( \sum_j a_j a_j^\dagger \) (or its complex conjugate).

From the DFT viewpoint, the breaking of the rotational symmetry implies that the density \( \rho(\vec{r}) \) can assume an intrinsic non-spherical shape, and the breaking of number symmetry implies that EDFs can also depend on a generalised density that is called abnormal density (or pairing tensor) and reads \( \kappa(\vec{r}) = \langle a(\vec{r})a(\vec{r}) \rangle \) (where \( a(\vec{r}) \) is the annihilation operator of a particle at point \( \vec{r} \) and \( a^\dagger(\vec{r}) \) is the corresponding creation operator). We remind the reader that the usual density that we have been dealing with so far reads \( \rho(\vec{r}) = \langle a^\dagger(\vec{r})a(\vec{r}) \rangle \) in second quantisation.

A full-fledged formulation of DFT with symmetry breaking goes beyond our scope here. The present Section can be considered an elementary introduction to specialised lectures on this topic, like Ref. [17].

10. – Extension to the time-dependent case

The extension of the HK theorem to the time-dependent case has been proposed by Runge and Gross in Ref. [83]. The Runge-Gross theorem guarantees that an exact functional exists, in principle, also for the time-dependent case. More precisely, given a
system whose behaviour is governed by an Hamiltonian

\[ H' = H + v_{\text{pert}}(t), \]

where the second term on the r.h.s. is a perturbing time-dependent potential (whose dependence on all degrees of freedom of the system is implicit), the theorem establishes a one-to-one correspondence between \( v_{\text{pert}}(t) \) and the time-dependent density \( \rho(t) \), that is,

\[ v_{\text{pert}}(\vec{r}, t) \leftrightarrow \rho(\vec{r}, t). \]

The proof of the Runge-Gross theorem is more subtle and involved than the proof of the static HK theorem that we have discussed in Sec. 2. This theorem constitutes the basis of time-dependent DFT (TDDFT). For a pedagogical introduction to the subject, the reader can consult Chapter 4 of Ref. [84].

TDDFT can also be approached within the Kohn-Sham scheme. In fact, the time-dependent density can be expressed in terms of time-dependent Kohn-Sham orbitals,

\[ \rho(\vec{r}, t) = \sum_j |\phi_j(\vec{r}, t)|^2, \]

and these orbitals must satisfy time-dependent Schrödinger equations of the type

\[ i\hbar \frac{\partial}{\partial t} \phi_j(\vec{r}, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{KS}}(\vec{r}, t) + v_{\text{pert}}(\vec{r}, t) \right] \phi_j(\vec{r}, t). \]

\( v_{\text{KS}}(\vec{r}, t) \) is the sum of three terms. The external potential \( v_{\text{ext}}(\vec{r}, t) \) and the Hartree potential \( v_{\text{Hartree}}(\vec{r}, t) \) are the straightforward generalisation of the first two terms at the l.h.s. of Eq. (9), where now the density is taken to be time-dependent. It is much less obvious how to extend the exchange-correlation potential defined in Eq. (9) to the time-dependent case, that is, how to determine what must be inserted in Eq. (52). Causality arguments play a role when one wishes to design a sensible strategy to build this potential: as pointed out in Ref. [85], the potential must not feel at time \( t \) the changes that the densities may undergo at later times, that is, at \( t' > t \). In fact, the rigorous proof of the Runge-Gross theorem implies a further key point that one should grasp, namely that the mapping (50) holds for a given initial condition at time \( t_0 \). In other terms, an exact exchange-correlation functional evaluated at time \( t \) should have memory of the whole previous history of the system for \( t' < t \).

In electronic systems, the construction of exchange-correlation functionals with memory is still in its infancy. Most calculations adopt the simple adiabatic approximation, in which also the exchange-correlation functional has the same form as the static one, Eq. (7), but is evaluated making use of the time-dependent density, viz.

\[ v_{\text{xc}}^{(\text{ALDA})}(\vec{r}, t) = v_{\text{xc}}[\rho(\vec{r}, t)], \]
where the label ALDA stays for adiabatic LDA. ALDA is basically the only option that has been so far explored in the nuclear case. Such approximation is expected to work better if the time scale of the perturbation is slow.

Given some assumption for $v_{KS}$, one can solve directly the time-dependent Kohn-Sham equations. A practical way is the following. If $h(t)$ is the sum of $v_{KS}$ plus the kinetic energy, the time evolution of the density can be written as

$$i\hbar \frac{d}{dt}\rho(t) = [h(t), \rho(t)].$$

Given an initial condition in which $\rho(t = t_0)$ is different from the stationary ground-state density, this latter equation can be solved by defining a time-evolution operator $\hat{U} \equiv e^{-i\int_0^t h(t') dt'}$, and by applying it to the density: starting from the density at time $t_0$, one can in fact write $\rho(t_0 + \Delta t) = \hat{U}\rho(t = t_0)$, where $\Delta t$ is an appropriate time step. This version of time-dependent DFT has been widely used. A useful introduction can be found in Refs. [86, 47], but many applications to nuclear vibrations [87], fusion processes [88], and heavy-ion reactions [89], among others, can be found in the recent literature.

The time-dependent equation (54) can be considered in the case of small external perturbations, namely it can be linearized. This linearization should be appropriate in the case of nuclear vibrations like the so-called giant resonances, and it is called linear response theory in general, and Random Phase Approximation (RPA) in the nuclear physics context. In this specific case, the adiabatic approximation should make sense as already pointed out in [83]; whether this approximation describes well specific physics cases, is a different and open question.

The derivation of RPA from Eq. (54) can be found in standard textbooks (see, e.g., Chapter 8 of [8]). We will not repeat it in detail here, but rather discuss the key ideas. If the perturbation $v_{pert}$ is small, it makes sense to assume it is harmonic,

$$v_{pert}(\vec{r}, t) = v_{pert}(\vec{r})e^{i\omega t} + \text{h.c.},$$

and then the density will display changes $\delta \rho(\vec{r}, t)$ that behave similarly as a function of time, that is,

$$\rho(\vec{r}, t) = \rho(\vec{r}) + \delta \rho(\vec{r}, t),$$
$$\delta \rho(\vec{r}, t) = \delta \rho(\vec{r})e^{i\omega t} + \text{h.c.},$$

where $\rho(\vec{r})$ is here the stationary ground-state density. RPA equations can be obtained by inserting (55) and (56) in (54), and retaining only terms that are linear in $\delta \rho$ or in $\delta h \equiv \frac{\partial h}{\partial \rho}\delta \rho$. If we go to limit of vanishing external perturbation, and if the final result is expressed on the basis of the Kohn-Sham orbitals, it reads

$$\left( \begin{array}{cc} A & B \\ -B & -A \end{array} \right) \left( \begin{array}{c} X \\ Y \end{array} \right) = \hbar \omega \left( \begin{array}{c} X \\ Y \end{array} \right).$$
This is an eigenvalue equation, and $\hbar \omega$ are the energies of the small-amplitude vibrations. For each of these modes, we have defined an eigenvector which is made up with the so-called forward-going and backward-going amplitudes $X_{mi}$ and $Y_{mi}$, respectively\(^{(9)}\). $X_{mi}$ ($Y_{mi}$) represents the probability amplitude that a transition from the orbital $i$ to $m$ ($m$ to $i$\(^{(10)}\)) contributes to the vibrational mode. The matrix elements that appear in Eq. (57) are defined by

\[
A_{mi,nj} = \delta_{ij} \delta_{mn} (\epsilon_m - \epsilon_i) + \int d^3r \ d^3r' \ \phi^*_m(\vec{r}) \phi^*_j(\vec{r}') \ \frac{\delta h(\vec{r})}{\delta \rho(\vec{r}')} \phi_i(\vec{r}) \phi_n(\vec{r}'),
\]

\[
B_{mi,nj} = \int d^3r \ d^3r' \ \phi^*_m(\vec{r}) \phi^*_n(\vec{r}') \ \frac{\delta h(\vec{r})}{\delta \rho(\vec{r}')} \phi_i(\vec{r}) \phi_j(\vec{r}'),
\]

where $\epsilon$ denotes the energies of the Kohn-Sham orbitals that have been introduced in Eq. (9). The physical interpretation of $\frac{\delta h(\vec{r})}{\delta \rho(\vec{r}')}$ is pretty intuitive: the changes of the density affect the single-particle effective operator $h$ (kinetic energy plus $v_{KS}$) and this, in turn, produces a rearrangement of the system. In other words, the system will perform harmonic oscillations around the ground-state that are governed by the residual force

\[
V_{\text{res}}(\vec{r},\vec{r}') \equiv \frac{\delta h(\vec{r})}{\delta \rho(\vec{r}')}.
\]

RPA equations can be also written in real-space instead than on a basis. This implementation allows a proper treatment of the continuum, but may become quite demanding if one deals with EDFs with many different terms. In fact, we have only mentioned the total density $\rho$ so far, but, according to the discussion of Sec. 6, realistic EDFs will bring in dependence on $\tau$, $\vec{\nabla} \rho$, $\vec{J}$ etc. Then, the variation of these densities will add new terms to the residual interaction (59), like $\frac{\delta h(\vec{r})}{\delta \rho(\vec{r}')}$ and so on.

A multitude of variants and applications of RPA exist in the literature. Part of it is reviewed, e.g., in Ref. [15]. We should add, in this context, that recently a new way of implementing RPA has been proposed [90], which is not yet discussed in standard textbooks and review papers. This method, called Finite Amplitude Method (FAM) realizes the above ideas of linear response in a quite straightforward way and has the advantage that the numerical implementation is far easier than those of standard methods.

11. Examples of RPA calculations

The best example of nuclear collective motion are the giant resonances, as we have already briefly mentioned. They are coherent modes, that dominate the response of nuclei in the energy region around $\approx 10-30$ MeV. Their properties are consistent with

\(^{(9)}\) Here, $i,j$ are used to label occupied orbitals and $m,n$ are used to label unoccupied orbitals.

\(^{(10)}\) Note that introducing the backward-going amplitudes is consistent with the linearity of the response, but implies relaxing the assumption that the ground-state is made up with the auxiliary orbitals filled up to the Fermi energy, and empty above this energy.
Density Functional Theory (DFT) for atomic nuclei: a simple introduction

the assumption of an elastic behaviour [91] and, in this respect, their integral properties are well described by RPA. Giant resonances carry different spatial angular momentum $L$, spin $S$, and isospin $T$. The states in which nucleons with opposite spin vibrate in phase (out of phase) are called electric (magnetic) resonances; if nucleons with opposite isospin, i.e. neutrons and protons, vibrate in phase (out of phase) one speaks of isoscalar (isovector) resonances.

We will mention only one of the multipoles in what follows. An external electromagnetic field excites the isovector dipole in a practically exclusive way. The response is dominated by the so-called isovector giant dipole resonance (IVGDR) at an energy around $80A^{-1/3}$: at that energy, the photon wavelength is much larger than the nuclear size and the associated electric field, that acts on the protons, is constant in space and thus consistent with a potential that is linear in the proton coordinates $\vec{r}_p$. It is very easy to check that if we take a potential of the type $e \sum_p \vec{r}_p$, and we transform it to the center-of-mass system, it becomes

$$\hat{O}_{IV\, dipole} = e N A \sum_p \vec{r}_p - e Z A \sum_n \vec{r}_n.$$  \hspace{1cm} (60)

In the center-of-mass system, protons and neutrons are displaced in opposite directions and the strong neutron-proton interaction acts as a restoring force.

In Fig. 6 we show strength functions resulting from RPA calculations with different Skyrme functionals (SGII from Ref. [97], SkI3 from Ref. [98] and SLy5 from Ref. [54]). Strength functions are defined by

$$S(E) = \sum_n |\langle n|\hat{O}(0)|\rangle|^2 \delta(E - \hbar \omega_n),$$  \hspace{1cm} (61)

where $n$ labels the solutions of Eq. (57), namely $\hbar \omega_n$ is an eigenvalue and $|n\rangle$ is the corresponding eigenvector, $|0\rangle$ is the ground-state, and $\hat{O}$ is a generic operator. Panels (a) correspond to the choice of the isovector operator (60), and the main IVGDR peak is compared with the photoabsorption result of Ref. [92], while the low-lying peak which is sometimes referred to as “pygmy” dipole resonance (PDR) is compared with the experimental findings of Refs. [93, 94]. Panels (b) show instead the response to the isoscalar dipole operator,

$$\hat{O}_{IS\, dipole} = \sum_i \left( r_i^3 - \frac{3}{5}(r_i^2)\hat{r}_i \right) Y_{1M}(\hat{r}_i).$$  \hspace{1cm} (62)

Details for this choice can be found in Ref. [96]. The result for the main resonance excited by this operator can be compared with the result of experiments like inelastic $(\alpha,\alpha')$ scattering, as we have done by taking the finding of [95]. The results in the figure seem to indicate that the low-lying dipole response has more isoscalar than isovector character.
Fig. 6. – Strength functions (61) corresponding to the isovector (a) and isoscalar (b) dipole response of $^{68}$Ni (left panels) and $^{208}$Pb (right panels) as a function of the excitation energy. The insets display on a larger scale the low-energy, or pygmy, region. The predictions obtained with different Skyrme functionals are depicted (cf. the main text). The results from Eq. (61) are averaged with Lorentzian functions having 1 MeV width. Black arrows indicate the experimental results from Refs. [92, 93, 94, 95]. Figure taken from Ref. [96].

Several textbooks have been devoted to the whole subject of nuclear giant resonances and reader can consult Refs. [99, 100]. The evolution of collective modes in neutron-rich nuclei is trated in Ref. [101].

12. – Limitations of EDFs

There is still debate on which are the intrinsic limitations of DFT in nuclear physics, and which are the practical limitations (due to the specific choices for the form of the EDF, and for the protocol to fit the parameters). Disentangling the two aspects is not easy.

The typical example of such debate is the issue with single-particle states. As we mentioned at the end of Sec. 5, the level density in nuclei is consistent with a value of the effective mass $m^*/m$ that lies around 0.7, but becomes close to 1 in the vicinity of the Fermi surface. Transfer experiments, although subject to a large amount of ambiguities, can provide access to the single-particle strength distributions in nuclei. Qualitatively, these experiments have shown that, close to the Fermi surface, these distributions display
dominant peaks, that is, are consistent with the existence of particle-like or hole-like levels; however, far from the Fermi surface, the single-particle strength is very fragmented. These patterns have been known for quite some time, and explained with the coupling between HF single-particle states and nuclear vibrations (particle-vibration coupling or PVC), as discussed at length in Ref. [45]. However, there are claims that, although PVC may be needed to explain single-particle fragmentation, the centroids of single-particle states must be obtained through improvements of current EDFs [102].

Even for observables that are the typical focus of nuclear DFT, like masses, we have mentioned in Sec. 7 that existing EDFs have errors that are typically around 1-2 MeV. Mass models that are more successful, and reduce this error below 1 MeV, include some terms that go outside the actual DFT philosophy. These terms correspond to vibrational or rotational correlations (cf. [69] and references therein).

There are other open questions that are related to the limits of current DFT implementations. MR-EDF has been shown to be a theory that is mathematically sound, and it has been successful in describing many low-lying nuclear spectra; still, pathologies in the results have shown up, as discussed in [103] and references therein. These pathologies have been associated with density-dependence in the Skyrme EDF, which on the other hand seems unavoidable if one wants to reconcile bulk properties and the effective mass. This is still a serious concern for practitioners. Another open question exists, regarding the pairing sector of the EDFs. In which way an EDF must depend on the abnormal density $\kappa(\vec{r})$, and possibly on its derivatives etc., is not clear yet. Links with an underlying theory of pairing in nuclei [104, 105] are still not enough. Proton-neutron pairing, as mentioned at the end of Sec. 9, is still not fully understood.

Last but not least, as briefly alluded to in Sec. 11, time-dependent DFT in the RPA implementation is known to be unable to reproduce the width of giant resonances, that is typically from few to several MeV. RPA can reproduce the so-called escape width, associated with particles decaying to the continuum, but not the remaining width, so-called spreading width. This letter is known to be accounted for in calculations that include PVC [106, 107, 108]. Whether functionals with memory effect may or not improve on this, is a further open question.

Several of these examples hint that vibrational correlations, pairing correlations, or other kinds of dynamical correlations, although in principle should be included in “exact” DFT, in practice are not included in existing EDFs. These limitations also call for a more serious confrontation between DFT and underlying theories, on the one hand, but also between DFT and many-body theories: this is not systematically carried on as it should, in the nuclear structure domain.

13. – Conclusions

We have tried to give the reader a brief survey about DFT, namely about its foundations and about the main specific features of nuclear DFT. Due to the scope of this volume, we have tried to give priority to pedagogical arguments, while we have simply provided references for all those detailed topics that are already well covered in the lit-
erature. As it has been stressed at the beginning, this contribution is meant to be an advanced, up-to-date introduction that serves mainly as an orientation for those interested in deepening their understanding of the large variety of DFT-related approaches.

The hope is to have been able to convince the reader that DFT has a number of advantages. Its basic principle is very transparent and intuitive: one writes the total energy as a function of the density, and chooses a way to minimise the energy! The HK theorem guarantees, then, that all bulk observables can be obtained: the density determines the shape of the system, the expectation values of relevant one-body operators (like electric quadrupole, or magnetic dipole, or higher multipole operators) as well as the total energy. The main advantage is that the applicability of DFT is very broad. All nuclei are amenable to a DFT description, except perhaps the very light ones. Moreover, there is a natural link with infinite nuclear matter and, thus, with the physics of compact objects like neutron stars.

After discussing DFT in electronic systems, we have, in fact, started our discussion by introducing nuclear DFT in uniform, symmetric nuclear matter. A sensible theory of such prototype system must display a mechanism for saturation; a good reproduction of the saturation point \(\rho_0 = 0.16 \text{ fm}^{-3}, \epsilon_0 = -16 \text{ MeV}\) is a necessary condition to describe also finite nuclei in a reasonable way. We have, then, provided arguments why naïve mean-field cannot be, in this respect, a sensible theory while DFT can. Of course, realistic EDFs should not simply provide a mechanism of nuclear saturation but should be flexible enough to account for surface properties, spin and isospin properties, and so on. Accordingly, we have discussed the appearance of different kinds of densities in existing EDFs.

A specific feature of finite nuclei is the appearance of spontaneous symmetry-breaking and restoration. Although specialised lectures exist on those topics, we have tried to give here an introduction through simple examples and arguments. In the case of deformed nuclei, the rotational symmetry is broken in the intrinsic reference frame, and rotations in the laboratory frame restore the symmetry. Within DFT, that has necessarily to be formulated in the intrinsic frame, as we have argued in Sec. 8, this implies the appearance of densities that are not rotationally invariant (that is, quadrupole or octupole moments as we have just stressed). A more intriguing example is that of pairing correlations that imply, instead, the appearance of the abnormal density or pairing tensor in the EDFs, breaking the particle number symmetry.

Last but not least, we have discussed the time-dependent case. The time-dependent DFT is still amenable to many improvements. Essentially all groups are using, so far, the adiabatic approximation. While this approximation, that corresponds to RPA in the nuclear structure theory language, has been successful in reproducing the main properties of the nuclear collective motion like the giant resonances, certainly examples of large-amplitude, slow motions exist in the nuclear case and call for more advanced approaches.

There are topics that we have not dealt with in this lecture and/or topics that have not been tackled yet by practitioners. One main issue is that, while in several papers the quest for a universal energy functional is advocated, still many different implementations of EDFs and even more variants based on different parameter sets are available on the
market. The situation in the case of electronic systems is, anyway, not much better [13]. Not only this fact makes DFT a domain that is believed to be for experts only but, more importantly, it raises the question if EDFs are systematically improvable or not. EFT has been proposed as a way out to this dilemma. However, a full derivation of DFT from EFT is not available yet.

Another aspect is the confrontation between DFT and many-body theory. The mapping of some many-body approximation into an EDF should be pursued more systematically, and is expected also to shed light on the present limitations of nuclear DFT. We have briefly mentioned the fact that DFT cannot describe the fragmentation of single-particle or collective states. This has been traditionally explained, in the nuclear context, by the coupling of single-particle and collective degrees of freedom (vibrations or rotations). Merging this description with up-to-date DFT, still represents a challenging task.

In summary, we may like to quote a saying by W. Kohn, and state that “DFT is an exactification of HF”; however, even though this statement may be true in principle, in practice many steps are still required to make the DFT description of the rich nuclear phenomenology more and more accurate.

** **

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