Review of Nuclear Density Functional Theory by G. Colo

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December 6, 2024

1 Abstract

Working to understand nuclear structure is referred to as "intricate, demanding, and sometimes painful" by G. Colo in "Nuclear Density Functional Theory" [1]. Nonetheless, progress continues, as 34 new nuclei were discovered in 2017 alone. Throughout the text, Colo stresses the complexities attached to exploring the range of nucleon density, as the properties vary widely. He claims Density Functional Theory (DFT) is the framework most capable of this exploration. Here, the mathematical ideas are quickly introduced, followed by a demonstration of the need for nuclear DFT, as well as how it is used to solve practical problems.

2 Quick Introduction to Density Functional Theory

The details of this section will reappear throughout the paper, with its purpose being to provide a quick summary of the "theory" of DFT in one place. (The book I used for a DFT introduction is [2].)
The many body Schrodinger equation is a critical tool for exploring quantum mechanical systems, as its solution, the many body wavefunction, allows the system to be probed. However, the analytical solution is attainable only in very specific cases, and approximations and alternative methods must be found. DFT is a mechanism to solve approximations of the many body Schrodinger equation, shown below.

$$\hat{H}\Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_n) = E\Psi(\boldsymbol{r}_1, ..., \boldsymbol{r}_n) \tag{1}$$

Instead of working from an exact, so called "generating", Hamiltonian, DFT's approach is to solve the many body Schrodinger heuristically. An effective Hamiltonian (H_{eff}) is built, and with the Hohenberg Kohn (HK) theorem, the energy is written as a functional of the particle density ρ,

$$E[\rho] = \langle\rho|\hat{H}_{\text{eff}}|\rho\rangle \tag{2}$$

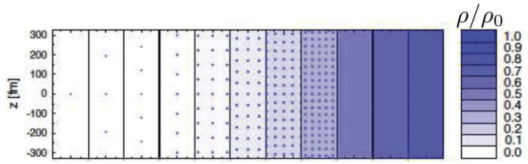
Nucleon ρ will be discussed further later, and is of key importance throughout the text. The minimization of this functional gives the ground state energy of the system, without truly touching the Schrodinger equation. From the ground state result, perturbations can be included to gain more information. In electronic structure theory, DFT has become a computational laboratory to explore material properties like bandgaps and absorption spectra. In nuclear physics, DFT performs a similar role, although requiring a step up (or more) in mathematical sophistication.

3 The Importance of Nucleon Density

Colo begins the introduction with the well known binding energy from the nuclear liquid drop model. For a nuclei with Z protons and N neutrons, this formula reads

$$BE(N, Z) = M(N, C)c^2 - Zm_pc^2 - Nm_nc^2 \tag{3}$$

with nuclear mass M, and proton and neutron masses m_p and m_n. This formula is used to find the saturation density of "typical medium-heavy nuclei of mass number $A = N + Z$", taking the value $\rho_0 \approx 0.16\text{fm}^{-3}$. Nuclei with $\rho \approx \rho_0$, to first order the nucleons may be treated as moving in a spherical average potential. However, this approximation fails terribly for the extremes of nucleon density, and Colo claims it is already a rough approximation for $\rho \approx \rho_0$. Clearly, there is a need to explore the entire range of nucleon density, as important phenomena arise throughout. On the low end, so called nucleon halo/skin occurs. Along the neutron drop line, protons are tightly bound to the neutrons, while many free neutrons remain. These free neutron wavefunctions can extend far from the nucleus, forming a nucleon halo or skin. At the high end, structures called neutron stars may form. Figure 1 demonstrates the structure of a neutron star as a function of ρ/ρ_0, showing neutron stars require usage of the entire range of nucleon density. One question that DFT helps answer is how does the symmetry energy (defined as the "energy per particle to change protons into neutrons starting from symmetric matter and moving to neutron matter") change the composition of the neutron star.



(a)

Figure 1: Visualization of neutron star composition as a function of ρ/ρ_0. The component (surface, outer crust, etc) are shown in the paper, but is not reproduced here.

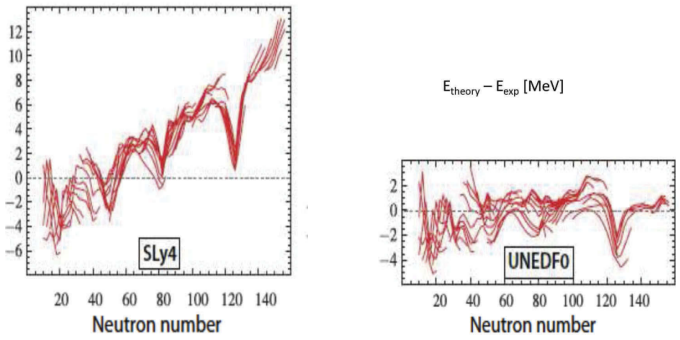
4 Nuclear Density Functional Theory, with Comparisons to the Electronic Case

4.1 QED vs QCD

The author claims somebody naive to nuclear physics may ask "Why don't we calculate nuclear properties starting from the fundamental theory of strong interactions?", going on to describe the differences between QCD, the theory of the strong interaction, and QED, the theory of the electromagnetic interaction. The difference is immense, with one root being the difference in coupling constants. The coupling constant in QED is $\alpha = \frac{1}{137}$, and allows perturbations at small energy scales. The coupling constant in QCD is close to 1, and does not allow the same perturbation opportunities. This problem shows why so many alternative methods, including DFT, are used. The text mentions an approach created by Weinberg, to use chiral effective field theory, proposing convergence to QCD at low energies. This seems one of the origins of the departure from working directly with QCD, and moving to effective Hamiltonians and energy density functionals (EDFs), which are now discussed..

4.2 Effective Hamiltonians and Energy Density Functionals

In electronic DFT, the mean field approximation is often used (so called Hartree-Fock). Instead of each electron accounting for every other electron, a "mean field" approximation is made that mimics each individual interaction. The mean field approximation is an example of introducing an effective potential, which replaces a density *dependent* interaction with one that is density *independent*. While this can have large benefit for electronic structures, Colo claims that after several decades of research, no density



(a) (b)

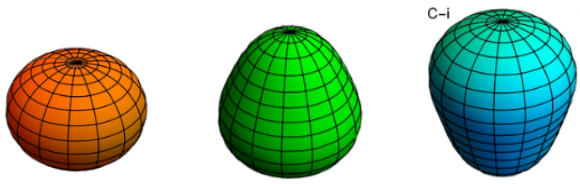
Figure 2: Comparison of the binding energy of atomic nuclei predicted by two different EDFs. The left using SLy4, the right using UNEDF0.

independent interaction provides realistic results for nuclear properties. So, effective Hamiltonians are built, from which the Schrodinger equation is thought of as a tool to build an EDF through

$$E = \langle \Psi | \hat{H}_{\text{eff}} | \Psi \rangle \tag{4}$$

The minimization of this functional gives the ground state of the system. (Here I want to talk about all the hard things that need to be included in these EDFs and maybe mention again that they are density dependent.) The author mentions various kinds of effective Hamiltonians/EDF's, and gives examples of some of the differences in performance between model. One example comparing two EDFs is shown in Figure 2. Figure 2a uses the so called Skyrme functional SLy4, and contains parameter fitting from magic nuclei only. Colo refers to Figure 2bs model as "more sophisticated", claiming that the ENEDF0 takes symmetry breaking into account. While ENEDF0 performs better than SLy4, neither fully match experimental data. The arches seen in either model are noted to be a common source of error for EDFs, and that these arches span what should be nuclear shells.

4.3 Symmetry Breaking

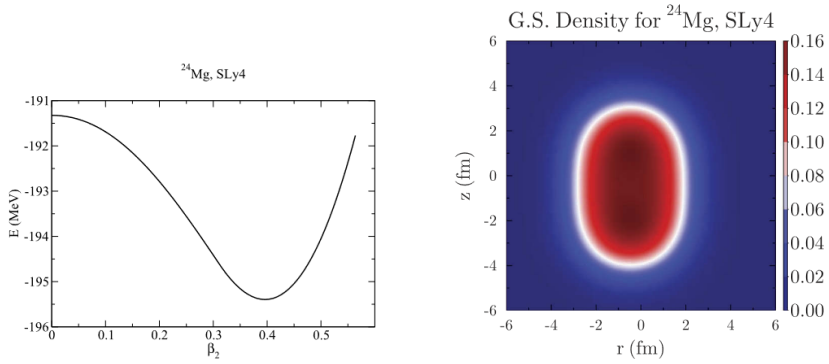


(a) (b) (c)

Figure 3: Examples of possible nucleon structure, with the second and third demonstrating symmetry breaking.

While using DFT to solve electronic problems is difficult, the author notes many differences portraying the heightened difficulty when dealing with the nuclear case. The first being that to current knowledge, the electron is a fundamental, point-like particle. Nucleons themselves are not, but are instead home to three fundamental constituents, called quarks. A direct consequence is that symmetry breaking must be taken into account when constructing effective Hamiltonian's in the nuclear case, whereas in the

electronic case, there is nothing *more* symmetric than a point particle. The author mentions so called quadrupole and octupole deformations as examples of nuclear symmetry breaking. Figure 3 demonstrates three of many possible configurations that need to be taken into account [3]. An interesting claim is made that super fluidity can be described in terms of symmetry breaking. One example of preferred symmetry breaking given in the text was done on ^{24}Mg, shown in Figure 4.



(a) (b)

Figure 4: (Left) Total energy vs deformation parameter β_2 of ^{24}Mg. (Right) Visualization of the ground state density.

Figure 4a shows the total energy against a deformation parameter β_2, essentially quantifying "how non-spherical am I?". Clearly, the minimum takes a non zero value of β_2, and the preferred energy state is one that breaks symmetry. Figure 4b visually demonstrating that the ground state breaks spherical symmetry.

4.4 Conclusion

Nuclear physics is an active field of research, and the author argues that DFT is the tool with the best handle on the wide range of nucleon density to be explored. There is a departure from generating Hamiltonians, with a move to effective Hamiltonians, from which an EDF is built and minimized to obtain the ground state energy. Applications of nuclear DFT were showcased, such as the neutron drip line, neutron stars, computing the ground state density, etc.

5 References

[1] G. Colò (2020) Nuclear density functional theory, Advances in Physics: X, 5:1, 1740061

[2] Giustino, F. (2020). Materials modelling using density functional theory: Properties and predictions. Oxford University Press.

[3] MohanMurthy, P., Silwal, U. and Winger, J.A. A survey of nuclear quadrupole deformation in order to estimate the nuclear MQM and its relative contribution to the atomic EDM. Interactions 245, 64 (2024)