

## Nuclear Density Functional Formalism

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### Introduction

The ground state properties of nuclei are commonly understood in the framework of mean field approximation, using effective density dependent nucleon-nucleon interaction, such as, for example, zero-range Skyrme forces [1] or finite range Gogny force [2], and using relativistic mean field (RMF) approach [3]. The parameters in these calculations are adjusted to reproduce properties of finite nuclei and nuclear matter, though in recent times data from theoretically determined neutron matter equation of state have also been used [4]. These calculations are successful in describing nuclear properties in spite of the uncertainties of the parameters of the effective forces which are still refined to account for the ever increasing set of nuclear data.

A completely different approach that is widely used to understand the many body physics in condensed matter, chemistry, and atomic physics, and has proved to be a very powerful tool there, is the Density Functional Theory (DFT) [5] in which the ground state density is the basic variable instead of wavefunction. In the recent time there is a lot of activity [6] in applying DFT to understand nuclear many body problem in spite of the fact that the applicability of DFT for self-bound systems is, so far, an unsettled problem. We show in this exploratory note how to build an energy density functional of DFT for nuclear many body problem using input from symmetric nuclear matter and neutron matter calculations.

### Formalism

The DFT is based on the Hohenberg-Kohn (HK) theorem, which states that the total en-

ergy of a many body system of fermions with a non-degenerate ground state can be expressed as a functional of the ground state density alone. The energy density functional reaches its variational minimum when evaluated with the exact ground state density. Kohn-Sham (KS) gave a practical method to calculate the density by solving a non-interacting Hartree-type problem with the same ground state density as the interacting system. In KS approach the energy density functional  $E[\rho]$  can be split into two parts,

$$E[\rho] = T_0[\rho] + V[\rho], \quad \text{with } V[\rho] = V_{int}[\rho] + V_{xc}[\rho], \quad (1)$$

where  $T_0[\rho]$ ,  $V_{int}[\rho]$  and  $V_{xc}[\rho]$  are respectively the kinetic energy, potential energy and exchange-correlation energy functionals.

Introducing an auxiliary set of orthonormal single particle orbitals,  $\psi_i(\mathbf{r})$ ,  $i = 1, \dots, A$ , with  $A$  being the number of particles, the density,  $\rho(\mathbf{r})$ , can be written as,

$$\rho(\mathbf{r}) = \sum_{i,s,t} |\psi_i(\mathbf{r}, s, t)|^2, \quad (2)$$

where  $s$  and  $t$  represent spin and isospin variables.

Employing variational procedure to minimise,  $E[\rho]$ , in terms of the orbitals instead of the density, a closed set of  $A$  Hartree-like equations containing an effective potential, which is functional derivative of  $V[\rho]$  with respect to local density  $\rho$ , are obtained for the ground state orbitals,  $\psi_i(\mathbf{r}, s, t)$ . A self-consistent procedure is used to solve these equations since the effective potential depends on the density, and in turn on the orbitals. The KS equations are exact, but those can be of some use if only  $V[\rho]$  is known accurately.

The kinetic energy functional,  $T_0[\rho]$ , and the potential energy functional,  $V_{int}[\rho]$ , can be written as,

$$T_0[\rho] = \frac{\hbar^2}{2m} \sum_{i,s,t} \int d^3r |\nabla \psi_i(\mathbf{r}, s, t)|^2, \quad (3)$$

$$V_{int}[\rho] = \frac{1}{2} \sum_{t,t'} \int d^3r d^3r' \rho_t(\mathbf{r}) V_{tt'}(\mathbf{r} - \mathbf{r}') \rho_{t'}(\mathbf{r}'), \quad (4)$$

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where  $V_{tt'}(\mathbf{r}-\mathbf{r}')$  represent finite range nucleon-nucleon potential. A simple Gaussian ansatz,

$$V_{tt'}(\mathbf{r}) = V_{tt'} \exp\left(-\frac{r^2}{r_0^2}\right), \quad (5)$$

can be made taking three open parameters,  $V_{p,p} = V_{n,n} = V_L$ ,  $V_{n,p} = V_{p,n} = V_U$ , and  $r_0$ . The parameters,  $V_L = -93.52$  MeV,  $V_U = -60.57$  MeV and  $r_0 = 1.05$  fm are obtained [7] by fitting to reproduce the binding energies of several nuclei nuclei.

Several approximation schemes are used for the most crucial part, the exchange-correlation energy functional,  $V_{xc}[\rho]$ , One of the widely used approximation schemes is the local density approximation. We can write  $V_{xc}[\rho]$  in this approximation as,

$$V_{xc}[\rho] = \int d^3r \rho(\mathbf{r}) E(\rho(\mathbf{r})), \quad (6)$$

where  $E(\rho(\mathbf{r}))$  can be taken as energy per nucleon corresponding to symmetric nuclear and neutron matter given in fig.(1), obtained following [8], in the framework of Brueckner-Hartree-Fock calculation with Bonn potential and including medium modification of the hadron parameters. These equations of state shown in fig.(1) correctly reproduce all the saturation observables and the symmetry energy.

We can write  $E(\rho(\mathbf{r}))$  as,

$$E(\rho(\mathbf{r})) = E_s(\rho)(1 - \beta) + E_n(\rho)\beta, \quad (7)$$

where  $E_s(\rho)$  and  $E_n(\rho)$  are the energy per nucleon for a given density  $\rho$  for symmetric nuclear and pure neutron matter, respectively. The density  $\rho$  and the asymmetry parameter,  $\beta$ , can be written as,

$$\rho = \rho_p + \rho_n, \quad \beta = \frac{\rho_n - \rho_p}{\rho}, \quad (8)$$

where  $\rho_n$  and  $\rho_p$  are neutron and proton densities.

### Summary and Conclusion

We have shown, in analogy to what is usually done in condensed matter physics, that the exchange correlation energy functional of KS-DFT inspired approach to nuclear many body

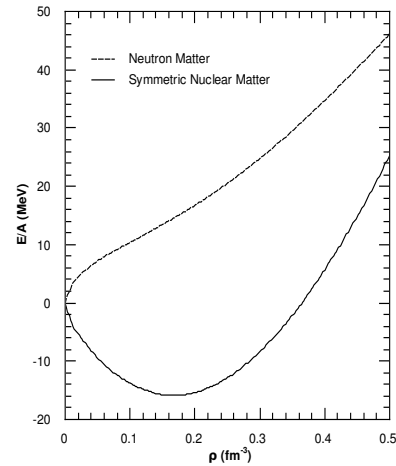


FIG. 1: Equation of state of symmetric nuclear and neutron matter obtained by the microscopic calculation .

problem can be obtained using the equation of state of symmetric nuclear and neutron matter. The energy density functional, however, is to be supplemented with spin-orbit part to do an actual calculation.

### References

- [1] D. Vautherin, D.M. Brink, Phys. Rev. **C5**,626 (1972).
- [2] J. Dechargé, D. Gogny, Phys. **C21**,1568 (1980).
- [3] P. Ring, Prog. Part. Nucl. Phys. **37**, 193 (1996) and references therein
- [4] E. Chabanat, P. Bonche, P. Haensel, J. Mayer and R. Schaefer, Nucl. Phys. **A627**, 710 (1997) ; **A635**, 231 (1998).
- [5] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
- [6] G. F. Bertsch, et al, Physical Review Letters **99**, 32502 (2007).
- [7] M. Baldo, P. Schuck, X. Vinas, Phys.Lett. **B663**, 390 (2008).
- [8] A. B. Santra, U. Lombardo, Int. Jnl. of Mod. Phys. **E18**, 1191 (2009).