

Review of mean-field theory Denis Lacroix GANIL-Caen International Joliot-Curie School 2011

Telescentral [1]

generalities

General remarks

- Nucleons are made of quarks
- The energy to excite quarks degrees of freedom (DOF) is much higher than the energy to excite nucleon DOF
- Nucleons are considered as elementary (point-like)
 Particles (low energy nucl. Phys. Point of view)

Nucleons are quantum interacting objects







generalities



From one to many nucleons

For one nucleon:

$$\phi_{\text{nucleon}} \equiv \phi(\mathbf{r}, \sigma, \tau)$$

For a N nucleon system:

$$\Psi(r_1,\cdots,r_{12},\cdots,r_{123},\cdots)$$

*spin, isospin omitted



[N! × size of nucleon space] DOF ...



Nuclei are among the most complex quantum mesoscopic systems



Exact (ab-initio) description can be made only in rare cases.

(see T. Papenbrock lecture)



Observation: emergence of single-particle aspects

e



(Courtesy O. Sorlin, EJC2009)



N=1

H.O. + L^2 + L.S



Summary : first dilemma Complexity

Observation: Separation energy, magic numbers,...

Separation energy: $S_n(A,Z) = B(A,Z) - B(A-1,Z)$

Nucleons behaves like independent particles in a single-particle field !!!



 $\Psi(r_1, \dots, r_{12}, \dots, r_{123}, \dots)$



 $\Psi = \mathcal{A}(\varphi_1(r_1), \cdots \varphi_N(r_N))$

$$\begin{cases} \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}) + f(\mathbf{r})\vec{l}.\vec{s} \\ \end{bmatrix} |\varphi_{\alpha}\rangle = \varepsilon_{\alpha}|\varphi_{\alpha}\rangle$$

Example : Wood Saxon potential $V(r) = \frac{V_0}{1 + \exp(\frac{r-R_0}{a})}$

Simplicity

Nuclei are quantum mesoscopic objects composed of fermions interacting through a strong highly repulsive interaction at short range Many aspects of nuclei can be fairly well understood assuming that nucleons behaves like independent particles in an external one-body field



-100

Gomes, Walecka and Weisskopf, Ann. Phys. (1958)

Why the independent particle works:

nn alone

fm



Ann. Phys. (1958)

Why the independent particle works:

Scattering theory, medium effects, ...



Why the independent particle works:

In medium Mean-Free Path

$\lambda~$ Mean-free path



Cugnon EJC2007

The second dilemma: failure of the Hartree-Fock theory

The infinite nuclear matter case

Basic aspects of Hartree-Fock theory

- (1) Start from \hat{H} And assume that $\Psi = \mathcal{A}(\varphi_1(r_1), \cdots \varphi_N(r_N))$
- (2) Minimize the action $\delta\left(\langle \Psi | \hat{H} | \Psi \rangle E \langle \Psi | \Psi \rangle\right) = 0$ with respect to single-particle deg. of freedom.

$$\Rightarrow h[\rho] |\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$
with $\rho = \sum_i |\varphi_i\rangle \langle \varphi_i$
and $h[\rho] = \frac{\partial E}{\partial \rho}$

3 Solve the HF equation self-consistently



The second dilemma

One-body density, Infinite nuclear matter, Saturation property



The second dilemma: failure of the Hartree-Fock theory

The infinite nuclear matter case



Density

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

$$\begin{aligned} |\mathbf{e}-\mathbf{particle state} \quad |\mathbf{k}\sigma\tau\rangle \\ \langle \mathbf{r}|\mathbf{p}\rangle &= \frac{1}{V^{1/2}}e^{i\mathbf{pr}/\hbar} \\ &= \frac{1}{V^{1/2}}e^{e^{i(k_xx+k_yy+k_zz)}} \\ k_i &= \frac{2\pi n_i}{L}, \quad i = x, y, z, \quad n_i = 0, \ \pm 1, \ \pm 2, \cdots \end{aligned}$$



The second dilemma: failure of the Hartree-Fock theory

Second Dilemma

Simplicity

Many aspects of nuclei can be fairly well understood assuming that nucleons behaves like independent particles in an external one-body field

Complexity

The natural approach to map a many-boby problem into a onebody theory (HF) does not work in nuclear physics

The Energy Density Functional approach



Basic aspects of Functional approach to nuclear systems

EDF has taken different names:	Skyrme/Gogny Hartree-Fock,
	Nuclear Density Functional Theory (DFT)
	Energy Density Functional (EDF)
What is Density Functional Theory ?	Relativistic Mean-Field

In its simplest form in DFT, the exact ground state of an N-body problem can be replaced by the minimization of an energy functional of the local one-body density $\rho(r)$. At the minimum, the energy and the density corresponds to the exact energy

$$\langle \Psi | \hat{H} | \Psi \rangle \Longrightarrow \mathcal{E}[\rho(r)]$$

Extensions:

- Introduction of auxiliary state $\Psi = \mathcal{A}(\varphi_1(r_1), \cdots \varphi_N(r_N))$ $\{\varphi_i\} \to \rho(r) \to \mathcal{E} \to U_{KS}(r) \to \{\varphi_i\}...$ Kohn, Sham, Phys. Rev. (1965) $\rho(r) = \sum_i |\varphi_i(r)|^2$ $h[\rho]|\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$ with $h[\rho] = \frac{\partial \mathcal{E}}{\partial \rho}$

Hohenberg, Kohn, Phys. Rev. (1965)

$$\mathcal{E} = \mathcal{E}[\rho(r), \nabla \rho, \Delta \rho, \tau, \dots]$$

$$\mathcal{E} = \mathcal{E}[\rho, \kappa...]$$

(and much more ...)

GGA, Meta GGA, ...

A primer to DFT, Lectures notes in Physics 620 (2003)

DFT with pairing

Oliveira et al, PRL (1988)

Time-dependent DFT

Runge, Gross PRL (1984)

Nuclear Energy Density Functional for pedestrian

Example 1 : empirical construction of EDF for nuclear matter

EDF from a simple perspective





$$E = \left\langle \frac{p^2}{2m} \right\rangle + U[\rho]$$

In nuclear matter:

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{3}{5} \left(\frac{3\pi^2}{2} \right)^{2/3} \rho^{5/3}$$

Fit with

$$U[\rho] = \sum_{n} c_n \rho^n$$



Coefficients contains many-body physics

Nuclear Energy Density Functional for pedestrian

Example 1 : empirical construction of EDF for finite nuclei

Observation



 $v(\mathbf{r}_1 - \mathbf{r}_2) = c_0 \delta(\mathbf{r}_1 - \mathbf{r}_2) \quad \Longrightarrow \quad U_{\mathrm{H}}(\mathbf{r}) = c_0 \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}') = c_0 \rho(\mathbf{r})$

Nuclear Energy Density Functional based on effective interaction

Illustration with the Skyrme Functional

Vautherin, Brink, PRC (1972)

$v(\mathbf{r}_1 - \mathbf{r}_2)$	$= t_0 \left(1 + x_0 \hat{P}_\sigma \right) \delta(\mathbf{r})$	central term
	$+ \frac{1}{2} t_1 \left(1 + x_1 \hat{P}_{\sigma}\right) \left[\mathbf{P}^{\prime 2} \ \delta(\mathbf{r}) + \delta(\mathbf{r}) \ \mathbf{P}^2\right]$	
	$+t_2 (1+x_2\hat{P}_{\sigma}) \mathbf{P}' \cdot \delta(\mathbf{r}) \mathbf{P}$	non local terms
	$+iW_0\sigma.\left[\mathbf{P}' imes \delta(\mathbf{r}) \mathbf{P} ight]$	spin orbit term
	$+rac{1}{6}t_3\left(1+x_3\hat{P}_{\sigma} ight) ho^{lpha}(\mathbf{R})\delta(\mathbf{r})$	density dependent term

Nuclear Energy Density Functional based on effective interaction

Illustration with the Skyrme Functional

Vautherin, Brink, PRC (1972)

$$\begin{aligned} v(\mathbf{r}_{1} - \mathbf{r}_{2}) &= t_{0} \left(1 + x_{0} \hat{P}_{\sigma} \right) \delta(\mathbf{r}) \\ &+ \frac{1}{2} t_{1} \left(1 + x_{1} \hat{P}_{\sigma} \right) \left[\mathbf{P}^{\prime 2} \, \delta(\mathbf{r}) + \delta(\mathbf{r}) \, \mathbf{P}^{2} \right] \\ &+ t_{2} \left(1 + x_{2} \hat{P}_{\sigma} \right) \mathbf{P}^{\prime} \cdot \delta(\mathbf{r}) \, \mathbf{P} \\ &+ i W_{0} \sigma. \left[\mathbf{P}^{\prime} \times \delta(\mathbf{r}) \, \mathbf{P} \right] \\ &+ \frac{1}{6} t_{3} \left(1 + x_{3} \hat{P}_{\sigma} \right) \rho^{\alpha}(\mathbf{R}) \, \delta(\mathbf{r}) \end{aligned}$$

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

$$\begin{split} \mathcal{H} &= \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} \\ &+ \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{Coull}} \end{split}$$

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

$$\mathcal{H}_{\rm so} = \frac{1}{2} W_0 \big[\mathbf{J} \cdot \nabla \rho + \mathbf{J}_p \cdot \nabla \rho_p + \mathbf{J}_n \cdot \nabla \rho_n \big]$$

$$\mathcal{H}_{sg} = -\frac{1}{16}(t_1x_1 + t_2x_2)\mathbf{J}^2 + \frac{1}{16}(t_1 - t_2)\left[\mathbf{J}_p^2 + \mathbf{J}_n^2\right]$$

Functional of $\rho, \rho_n, \rho_p, \tau, \tau_n, \tau_p, \mathbf{J}, \dots$ Around 10-14 parameters to be adjusted

Nuclear Energy Density Functional based on effective interaction

Constraining the functional

See for instance, Meyer EJC1997

Vautherin, Brink, PRC (1972)

$$\begin{split} v(\mathbf{r}_{1} - \mathbf{r}_{2}) &= t_{0} \left(1 + x_{0} \hat{P}_{\sigma} \right) \delta(\mathbf{r}) \\ &+ \frac{1}{2} t_{1} \left(1 + x_{1} \hat{P}_{\sigma} \right) \left[\mathbf{P}^{\prime 2} \, \delta(\mathbf{r}) + \delta(\mathbf{r}) \, \mathbf{P}^{2} \right] \\ &+ t_{2} \left(1 + x_{2} \hat{P}_{\sigma} \right) \mathbf{P}^{\prime} \cdot \delta(\mathbf{r}) \, \mathbf{P} \\ &+ i W_{0} \sigma. \left[\mathbf{P}^{\prime} \times \delta(\mathbf{r}) \, \mathbf{P} \right] \\ &+ \frac{1}{6} t_{3} \left(1 + x_{3} \hat{P}_{\sigma} \right) \rho^{\alpha}(\mathbf{R}) \, \delta(\mathbf{r}) \end{split}$$

Tensor interaction

$$v^{t}(\mathbf{r}) = \frac{1}{2}t_{e}\{[3(\sigma_{1} \cdot \mathbf{k}')(\sigma_{2} \cdot \mathbf{k}') - (\sigma_{1} \cdot \sigma_{2})\mathbf{k}'^{2}]\delta(\mathbf{r}) \\ + \delta(\mathbf{r})[3(\sigma_{1} \cdot \mathbf{k})(\sigma_{2} \cdot \mathbf{k}) - (\sigma_{1} \cdot \sigma_{2})\mathbf{k}^{2}]\} \\ + t_{o}[3(\sigma_{1} \cdot \mathbf{k}')\delta(\mathbf{r})(\sigma_{2} \cdot \mathbf{k}) - (\sigma_{1} \cdot \sigma_{2})\mathbf{k}' \cdot \delta(\mathbf{r})\mathbf{k}]\}$$





Otsuka et al, PRL95 (2005)

Infinite nuclear matter and Nuclear Masses





Energy Density Functional based on effective interaction

Charge density



Density Functional theoryAre firstly optimal for:(i) Ground state energy(ii) Local one-body density

And it does it very well...

Success

Ground state energy





To improve the functional one can:

Add new terms: better isospin dependence, tensor,...)

Make better fit on precise containing new information





Use symmetry breaking in Functional theory

Let us restart from the nuclear Hamiltonian

$$H = \sum_{ij} \langle i|T|j\rangle a_i^+ a_j + \frac{1}{2} \sum_{ijkl} \langle ij|v_{12}|lk\rangle a_i^+ a_j^+ a_l a_k$$

A symmetry is conserved if the Hamiltonian commute with the generator of the group of Transformation associated with this symmetry: [H,G]=0

Some symmetries that are respected by the nuclear Hamiltonian:



Fingerprints of spontaneous symmetry breaking and intrinsic frame



Theoretical approach to symmetry breaking



with $\hat{h}(\hat{x}_i) = \frac{\hat{p}_i^2}{2m_i} + C\hat{x}_i^2$ $\stackrel{b_i \to 0}{\Longrightarrow} \varphi_i(x_i) \propto e^{\frac{ip_i x_i}{\hbar}}$

Success of EDF and broken symmetries

Z=24

Z-22

Z=20

Z=16

Z-14





Symmetry restoration

Third dilemma

The many-body state respect all symmetries of H in the lab. frame

MB states should ultimately have good quantum numbers

EDF uses symmetry breaking to grasp correlation which are not easy to get without symmetry breaking

MB states do not have good quantum numbers

Symmetry Restoration : the rotation case



Some example of symmetry breaking restoration



Configuration Mixing within EDF

EDF: status in nuclear structure studies



Dilemma: While data contains "fingerprints of symmetry breaking" the theory should be Symmetry conserving



Configuration Mixing within EDF

Interplay between single-particle and collective degrees of freedom





Configuration Mixing within EDF

EDF: status in nuclear structure studies





Bender, Duguet, Heenen, Lacroix, arXiv:1011.4047

What we ask to a modern mean-field theory ?



And much more...

EDF, from ground state to thermodynamics, to dynamics



Nuclear Reactions

Interplay between nuclear reaction and nuclear structure





Example of study: the onset of dissipation



Simenel, Avez, Lacroix, arXiv:0806.2714

A unified theory for nuclear structure, reactions and stars



Strategy 1: exploring unknown region



 $\operatorname{Radius} \times \operatorname{Pressure}^{-1/4} \simeq \operatorname{cte}$

Lattimer et al, Phys. Rep. (2000)

 Measurement of neutron star radii constraint the asymmetry energy

Cooling of proto-neutron star

Exotic phases

A unified theory for nuclear structure, reactions and stars

Range of application



A unified theory for nuclear structure, reactions and stars



Towards non-empirical EDF

