**Nuclear Density Functional Theory for Astrophysics** 

PART I – Nuclear properties and excitations

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# THE CHART OF THE NUCLIDES



How are the elements in the universe produced?

#### Big-bang nucleosynthesis



# Hydrostatic nucleosynthesis in stars

- Hydrogen burning continues until the fuel is spent, leading to contraction of the star and higher temperatures.
- Burning cycles with different fuel continue (depending on mass of the star) all the way to iron!





Iron and nickel have two most stable isotopes – combining them into even heavier nuclei would consume more energy than it would provide.

Nucleosynthesis of elements heavier than Fe:

• Neutron capture and successive β-decay







#### NUCLEAR THEORY

- The goal: understanding the properties of nuclei for the synthesis of elements and properties of stars
- Nuclear theory approaches (microscopic)
  - Ab initio models
  - Interacting shell model
  - energy density functionals
  - ...
- Method of choice: Density functional theory allows a consistent approach to nuclear matter, finite nuclei and nuclear processes along the nuclide map



 Mainly based on mean field models (Skyrme, Gogny, relativistic)

# DENSITY FUNCTIONAL THEORY



# **DENSITY FUNCTIONAL THEORY (DFT)**



From: nobelprize.org

- **Walter Kohn** The Nobel Prize in Chemistry 1998 ٠  $\diamond$  "for his development of the density-functional theory"
- Kohn, Hohenberg, Sham, ... •
- Successful applications of DFT in chemistry and condensed-matter physics
- Within the DFT it is not necessary to account for every electron's movement. ٠ Instead, one could look at the average density of electrons in the space.
- DFT shifts the emphasis from the individual wave functions to the density

- Hohenberg-Kohn theorem the exact energy of a quantum many body system is a functional  $E(\rho)$  of the local density  $\rho(\vec{r})$
- Ground state density and other ground state observables are obtained by minimizing a suitable energy functional  $E(\rho)$

# The strategy in the nuclear EDF approach:

- Establish an optimal EDF based on some effective nuclear interaction
- the nuclear energy functional is so far phenomenological and not connected to realistic NN-interaction
- Constrain the empirical parameters of the functional and its validation using available many body observables such as masses, radii, pseudo-data, etc.
- Complicated many body effects are encoded in the empirical constants
- EDF valid through the entire chart of nuclides, light and heavy, spherical and deformed
- Develop theory frameworks for applications of the functional to address various static and dynamic nuclear phenomena, processes, nuclear equation of state, neutron stars,
   ...

# ENERGY DENSITY FUNCTIONAL (EDF)



#### SELF-CONSISTENT RELATIVISTIC MEAN FIELD MODEL

- The implementation of density functional theory in the relativistic framework in terms of self-consistent relativistic mean-field model
- The basis is an effective Lagrangian with relativistic symmetries



System of Dirac nucleons coupled by the exchange meson and the photon fields



#### Extensions:

• pairing correlations (Relativistic Hartree-Bogoliubov model)

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_m + \mathcal{L}_{int}$$

- the Lagrangian of the free nucleon:  $\mathcal{L}_N = \bar{\psi} (i \gamma^\mu \partial_\mu m) \psi$
- the Lagrangian of the free meson fields and the electromagnetic field:

$$\mathcal{L}_{m} = \frac{1}{2} \partial_{\mu} \sigma \partial^{\mu} \sigma - \frac{1}{2} m_{\sigma}^{2} \sigma^{2} - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_{\omega}^{2} \omega_{\mu} \omega^{\mu} - \frac{1}{4} \vec{R}_{\mu\nu} \vec{R}^{\mu\nu} + \frac{1}{2} m_{\rho}^{2} \vec{\rho}_{\mu} \vec{\rho}^{\mu} - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

• minimal set of interaction terms:

$$\mathcal{L}_{int} = -\bar{\psi}\Gamma_{\sigma}\sigma\psi - \bar{\psi}\Gamma^{\mu}_{\omega}\omega_{\mu}\psi - \bar{\psi}\vec{\Gamma}^{\mu}_{\rho}\vec{\rho}_{\mu}\psi - \bar{\psi}\Gamma^{\mu}_{e}A_{\mu}\psi.$$

• with the vertices:  $\Gamma_{\sigma} = g_{\sigma}, \quad \Gamma^{\mu}_{\omega} = g_{\omega}\gamma^{\mu}, \quad \vec{\Gamma}^{\mu}_{\rho} = g_{\rho}\vec{\tau}\gamma^{\mu}, \quad \Gamma^{m}_{e} = e\frac{1-\tau_{3}}{2}\gamma^{\mu}$ 

$$\partial_{\mu} \frac{\partial L}{\partial (\partial_{\mu} q_k)} - \frac{\partial L}{\partial q_k} = 0.$$

- Dirac equation (nucleons)
- Klein-Gordon eqs. (meson fields)
  - Self-consistent solution

#### SELF-CONSISTENT RELATIVISTIC MEAN FIELD MODEL

- Effective density dependence of the model motivated by ab-initio calculations
- Density dependent meson-nucleon couplings



Effective interactions with mediumdependent couplings:



# COUPLING PARAMETERS: gσ(ρ), gω(ρ), g<sub>ρ</sub>(ρ)

- Relativistic point coupling model
- The basis is an effective Lagrangian with four-fermion (contact) interaction terms; isoscalar-scalar, isoscalar-vector, isovector-vector, derivative term

$$\mathcal{L} = \bar{\psi}(i\gamma \cdot \partial - m)\psi - \frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^{\mu}\psi)(\bar{\psi}\gamma_{\mu}\psi) - \frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^{\mu}\psi)(\bar{\psi}\vec{\tau}\gamma_{\mu}\psi) - \frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma \cdot A\frac{(1-\tau_3)}{2}\psi$$

- many-body correlations encoded in density-dependent coupling functions that are motivated by microscopic calculations but parameterized in a phenomenological way
- Extensions: pairing correlations in finite nuclei
  - Relativistic Hartree-Bogoliubov model
  - (e.g. with separable form of the pairing interaction Y. Tian, Z. Y. Ma, P. Ring, PLB 676, 44 (2009).)

#### SELF-CONSISTENT RELATIVISTIC MEAN FIELD MODEL

 Density dependence of the couplings - To establish the density dependence of the couplings one could start from a microscopic equation of state of symmetric and asymmetric nuclear matter.

$$\alpha_i(\rho) = a_i + (b_i + c_i x)e^{-d_i x} \qquad (i \equiv S, V, TV)$$
$$x = \rho/\rho_{sat}$$

• 12 model parameters:

$$egin{aligned} & a_s, b_s, c_s, d_s \ & a_v, b_v, d_v \ & b_{TV}, d_{TV} \ & \delta_s \ & g_n, g_p \end{aligned}$$

- isoscalar-scalar
- isoscalar-vector
- isovector-vector
- derivative term
- pairing correlations (strength parameters)

#### CONSTRAINING THE FUNCTIONAL

- The model parameters  $\mathbf{p} = (p_1, ..., p_n)$  are constrained directly by many-body observables using  $\chi^2$  minimization

$$\chi^{2}(\boldsymbol{p}) = \sum_{i=1}^{m} \left( \frac{\mathcal{O}_{i}^{\text{theo.}}(\boldsymbol{p}) - \mathcal{O}_{i}^{\text{ref.}}}{\Delta \mathcal{O}_{i}^{\text{ref.}}} \right)^{2}$$

• Calculated values can be compared to experimental, observational, and pseudo-data



properties of finite nuclei – binding energies, charge radii, diffraction radii, surface thicknesses, pairing gaps, etc.,...

 nuclear matter properties – equation of state, binding energy and density at the saturation, symmetry energy J & L, incompressibility...



 Isovector channel of the EDF is weakly constrained by exp. data such as binding energies and charge radii. Possible observables for the isovector properties: *neutron radii, neutron skins, dipole polarizability, pygmy dipole strength, neutron star radii*

#### NUCLEAR MATTER EQUATION OF STATE AND SYMMETRY ENERGY

Nuclear matter equation of state:

$$E(\rho, x) = E_{SNM}(\rho) + E_{sym}(\rho)(1 - 2x)^2 + \dots$$

$$\rho = \rho_n + \rho_p \ , x = \rho_p / \rho$$

Symmetry energy term:

$$E_{sym}(\rho) \equiv S_2(\rho) = J - L\epsilon + \dots$$
  

$$\epsilon = (\rho_0 - \rho) / (3\rho_0)$$
  

$$L = 3\rho_0 \frac{dS_2(\rho)}{dr}|_{\rho_0}$$

J – symmetry energy at saturation density L – slope of the symmetry energy (related to the pressure of neutron matter)



#### COVARIANCE ANALYSIS IN THE FRAMEWORK OF EDFs

• The quality of X<sup>2</sup> minimization is an indicator of the statistical uncertainty



• Assume that  $\chi^2$  is a well behaved hyper-function of the parameters around their optimal value  $\mathbf{p}_0, \partial_{\mathbf{p}}\chi^2(\mathbf{p}) \mid_{\mathbf{p}=\mathbf{p}_0} = 0$ 

- Near the minimum,  $\chi^2\,$  can be approximated by a Taylor expansion as an hyper-parabola in the parameter space

$$\chi^2(\boldsymbol{p}) - \chi^2(\boldsymbol{p}_0) \approx \frac{1}{2} \sum_{i,j}^n (p_i - p_{0i}) \partial_{p_i} \partial_{p_j} \chi^2(p_j - p_{0j})$$

Curvature matrix:

Covariance between two quantities A and B:

$$\mathcal{M}_{ij} = \frac{1}{2} \partial_{p_i} \partial_{p_j} \chi^2 |_{\mathbf{p}_0} \qquad \overline{\Delta A \, \Delta B} = \sum_{ij} \partial_{p_i} A(\hat{\mathcal{M}}^{-1})_{ij} \partial_{p_j} B$$

• Variance  $\overline{\Delta^2 A}$  and  $\overline{\Delta^2 B}$  define statistical uncertainties of each quantity.

#### **Pearson product-moment correlation coefficient** provides a measure of the correlation (linear dependence) between two variables A and B.

$$c_{AB} = \frac{|\overline{\Delta A \, \Delta B}|}{\sqrt{\overline{\Delta A^2} \, \overline{\Delta B^2}}}$$

#### CORRELATIONS: NUCLEAR MATTER vs. PROPERTIES OF NUCLEI



#### NEUTRON SKINS AND DENSITY DEPENDENCE OF THE SYMMETRY ENERGY

- In nuclei, neutron densities are equally important as charge densities, but more difficult to assess
- The thickness of the neutron skin  $r_{np} = r_n r_p$  depends on the pressure of neutron matter  $P_{PNM} \sim L$ : the size of  $r_{np}$  increases with pressure as neutrons are pushed out against surface tension
- The same pressure supports a neutron star against gravity (models with thicker neutron skins - neutron stars with larger radii)
- The pressure of neutron matter P<sub>PNM</sub> ~ L is poorly constrained

Large theoretical uncertainties in the energy per particle as a function of the density for pure neutron matter.



#### NEUTRON SKINS AND DENSITY DEPENDENCE OF THE SYMMETRY ENERGY



# NEUTRON SKINS AND DENSITY DEPENDENCE OF THE SYMMETRY ENERGY

- An accurate measurement of the neutron radius / neutron skin thickness in <sup>208</sup>Pb may have important implications for understanding the symmetry energy and the properties of neutron stars
- Abrahamyan et al. PRL 108, 112502 (2012) parity violating electron scattering

Lead Radius Experiment (PREx) @ JLab

 $R_n - R_p = 0.33^{+0.16}_{-0.18}$ 



From nuclear collective motion:

Various modes of excitation provide constraints on the neutron skin thickness, e.g.

- Pygmy dipole resonances: A. Carbone et al., PRC 81, 041301(R) (2010)
   A. Klimkiewitz et al., PRC 76, 051603(R) (2007)
- Dipole polarizability: A. Tamii et al., PRL 107, 062502 (2011)

D.M. Rossi et al., PRL 111, 242503 (2013)

- Anti-analog GDR: A. Krasznahorkay et al., PLB 720, 428 (2013)
- Quadrupole resonances: S.S. Henshaw, M.W. Ahmed, G. Feldman et al, PRL 107, 222501 (2011)

• ...

Other approaches: pion photoproduction Taubert et al. PRL 112, 242502 (2014), etc.

# CONSTRAINING THE SYMMETRY ENERGY

Isovector dipole transition strength – calculations are based on the same set of energy density functionals which vary the symmetry energy properties



#### CONSTRAINING THE SYMMETRY ENERGY



- The same set of DD-ME interactions used in the analysis based of various giant resonances and pygmy strengths (consistent theory !)
- Excellent agreement, except for the AGDR new measurements are needed for the AGDR

# THE NUCLEAR MATTER INCOMPRESIBILITY

- Nuclear matter incompressibility  $K_{nm} = 9\rho_0^2 \frac{d^2}{d\rho^2} \frac{E}{A}|_{\rho=\rho_0}$
- It can be determined from the energies of compression mode in nuclei: Isoscalar Giant Monopole Resonance (ISGMR)



• ISGMR energies are extracted from inelastic scattering of α-particles

$$E_{ISGMR} = \hbar \sqrt{\frac{K_A}{m \langle r^2 \rangle}}$$
 (for nuclei)

- Strategy to reach K<sub>nm</sub> (nuclear matter) :
- 1) Build the energy density functional (EDF), each parameterization corresponds to a  $K_{nm}$
- 2) Calculate ISGMR excitation energy using the same EDF (e.g., RPA)
- 3) The K<sub>nm</sub> value associated with the EDF that best describes the experimental ISGMR energy is considered as the "correct" one.

#### THE NUCLEAR MATTER INCOMPRESIBILITY

Using inelastic  $\alpha$  scattering the strength distributions of the isoscalar giant monopole resonances (ISGMR) have been measured in nuclei

e.g., D. Patel et al., Phys. Lett. B 726, 178 (2013)



| Target            | $E_{ISGMR}$ (MeV) |  |                  |                  | $\Gamma_{ISGMR}(MeV)$ | $\sqrt{m_1/m_{-1}} ({ m MeV})$ |                          | $E_{ISGMR}A^{1/3}$ (MeV) |                                  |
|-------------------|-------------------|--|------------------|------------------|-----------------------|--------------------------------|--------------------------|--------------------------|----------------------------------|
|                   | This work         | $\mathrm{RCNP}\text{-}\mathrm{U}^{\mathrm{a}}$ | Texas $A\&M^b$   | KVI <sup>c</sup> | This work             | This work                      | Pairing+MEM <sup>d</sup> | This work                | $\operatorname{Pairing+MEM^{d}}$ |
| <sup>204</sup> Pb | $13.8 {\pm} 0.1$  | -  | -                | -                | $3.3{\pm}0.2$         | $13.7{\pm}0.1$                 | 13.4                     | $81.2{\pm}0.6$           | 78.9                             |
| <sup>206</sup> Pb | $13.8 {\pm} 0.1$  | -  | -                | $14.0\ \pm 0.3$  | $2.8{\pm}0.2$         | $13.6{\pm}0.1$                 | 13.4                     | $81.5{\pm}0.6$           | 79.1                             |
| $^{208}$ Pb       | $13.7{\pm}0.1$    | $13.5{\pm}0.2$                                 | $13.91{\pm}0.11$ | $13.9{\pm}0.3$   | $3.3{\pm}0.2$         | $13.5{\pm}0.1$                 | 14.0                     | $81.2{\pm}0.6$           | 82.9                             |

#### NEUTRON STAR PROPERTIES

• Mass-radius relations of cold neutron stars for different EOS – observational constraints on the neutron star mass rule out many models for EOS.



#### CONSTRAINTS ON THE NUCLEAR EOS BEYOND SATURATION

- The knowledge on the nuclear matter equation of state (EOS) beyond the saturation density  $\rho_0$  is limited
- Some constraints on the EOS are possible from heavy ion collisions
- The FOPI (GSI) detector data on elliptic flow in Au+Au collisions between 0.4 and 1.5A GeV were used to establish empirical constraints on the nuclear EOS

   A. Le Fèvre, Y. Leifels, W. Reisdorf, J. Aichelin, Ch. Hartnack, arXiv:1501.05246 (2015).

• FOPI-IQMD (transport code) provides limits to the symmetric nuclear matter EOS up to  $2\rho_0$ 



# NUCLEAR MASSES

• Description of experimental data on masses: DD-ME2, DD-PC1, DD-MEδ, NL3\*



# NUCLEAR MASSES

• Relative accuracies in description of the masses



#### NUCLEAR LANDSCAPE WITH RELATIVISTIC EDFs

**Systematical model uncertainties** – limitations of the model, deficient parametrizations, wrong assumptions, and missing physics due to our lack of knowledge.

 These uncertainties are difficult to estimate – systematic errors can be estimated e.g., by exploring the spread - difference between maximal and minimal values obtained for a set of EDFs: DD-ME2, DD-PC1, DD-MEδ, NL3\*

$$\Delta E(Z,N) = |E_{max}(Z,N) - E_{min}(Z,N)|$$



#### NUCLEAR LANDSCAPE WITH RELATIVISTIC EDFs

 Limits of nuclear landscape – two-proton and two-neutron drip lines calculated with different relativistic EDFs: DD-ME2, DD-PC1, DD-MEδ, NL3\*



#### SYSTEMATIC UNCERTAINTIES : NEUTRON SKIN THICKNESS

 Electric dipole polarizability α<sub>D</sub> and neutron skin thickness (r<sub>skin</sub>) for <sup>208</sup>Pb using both nonrelativistic and relativistic EDFs:





By using only models consistent with measured  $\alpha_D$  (48 EDFs  $\rightarrow$  25 EDFs), systematic model uncertainty in  $r_{skin}$  is reduced.

Model averaged value:

 $r_{skin}(^{208}Pb) = (0.168 \pm 0.022) \text{ fm}$ 

J. Piekarewicz, et al., PRC 85, 041302 (R) (2012)

#### STATISTICAL UNCERTAINTIES IN THE NUCLEAR BINDING ENERGIES

 The evolution of statistical uncertainties of the nuclear binding energies within isotope chains (RNEDF1)



- The quality of X<sup>2</sup> minimization of the EDF parameters to exp. data is an indicator of the statistical uncertainty
- curvature matrix

$$\mathcal{M}_{ij} = \frac{1}{2} \partial_{p_i} \partial_{p_j} \chi^2 |_{\mathbf{p}_0}$$

 Constraint on the dipole polarizability / symmetry energy improves the isovector properties of the EDF Towards a universal relativistic nuclear energy density functional for astrophysical applications – RNEDF1 (N.P., M. Hempel et al. 2016)

The strategy to constrain the functional (relativistic point coupling model)

- Adjust the properties of 72 spherical nuclei to exp. data (binding energies (△=1 MeV), charge radii (0.02 fm), diffraction radii (0.05 fm), surface thickness (0.05 fm))
- Improve description of open-shell nuclei by adjusting the pairing strength parameters to empirical paring gaps (n,p) (0.14 MeV)
- constrain the symmetry energy  $S_2(\rho_0)=J$  (2%) from exp. data on dipole polarizability (<sup>208</sup>Pb) A. Tamii et al., PRL 107, 062502 (2011) + update (2015).
- constrain the nuclear matter incompressibility K<sub>nm</sub> (2%) from exp. data on ISGMR modes (<sup>208</sup>Pb); D. Patel et al., PLB 726, 178 (2013).

# ... the strategy to constrain the functional

- constrain the equation of state using the saturation point (ρ<sub>0</sub>) and point at twice the saturation density (2ρ<sub>0</sub>) from heavy ion collisions (FOPI-IQMD) (10%)
   A. Le Fevre et al., arXiv:1501.05246v1 (2015)
- constrain the maximal neutron star mass by solving the Tolman-Oppenheimer-Volkov (TOV) equations and using observational data (slightly larger value M<sub>max</sub>=2.2M<sub>☉</sub>(5%); J. Erler. et al., PRC 87, 044320 (2013).)
   J. Antoniadis, et al. Science 340, 448 (2013); P. B. Demorest et al., Nature 467, 1081 (2010)
- the fitting protocol is supplemented by the covariance analysis

   calculation of the curvature matrix, correlations, statistical uncertainties

# RNEDF1: DEVIATIONS FROM THE EXP. DATA



# **RNEDF1: NUCLEAR MATTER PROPERTIES**



#### RNEDF1: COMPRESSIBILITY, SYMMETRY ENERGY





#### MASSES: FROM FINITE NUCLEI TOWARD THE NEUTRON STAR

Nuclear binding energies (calc. – exp.) - Including deformation (axial symmetry) Neutron star mass-radius relationship



#### **RNEDF1: ISOTOPE AND ISOTONE CHAINS**



#### RNEDF1: NEUTRON SKIN THICKNESS IN <sup>208</sup>Pb



 $(γ,π^0)$ : C.M. Tarbert et al., PRL 112, 242502 (2014) PREX: S. Abrahamyan et al., PRL. 108, 112502 (2012) (p,p'): A. Tamii et al., PRL 107, 062502 (2011) (p,p) J. Zenihiro et al., PRC 82, 044611 (2010) Antipr. at.: B. Kłos et al., Phys. Rev. C 76, 014311 (2007). LAND (PDR): A. Klimkiewicz et al., PRC 76, 051603 (2007). SV-min: P.G. Reinhard et al. SLy5-min: X. Roca-Maza, G. Colò et al. FSUGold: J. Piekarewicz et al. DDME-min1: N.P. et al.