

From nucleons to neutron stars in the unifying framework of energy density functional theory Panagiota Papakonstantinou

October 28, 2024 Dense Nuclear Matter Equation of State from Theory and Experiments FRIB, East Lansing MI, USA

Contents

01 Introduction

Nuclei-nucleons-nuclear matter Nuclear EDF

02 Nuclear EDFT news

KIDS framework Correlation studies

03 Recent developments 04

Density regimes Beyond one-body picture **Conclusion**

Status summary

Contents

01 Introduction

Nuclei-nucleons-nuclear matter Nuclear EDF

Energy density functional theory boils down to:

❑ The energy of a system is a function of the density [distribution].

Hohenberg-Kohn and Kohn-Sham theorems

- ❑ One may as well use mean-field theory: Consider non-interacting particles in a single-particle potential such that the energy and density of the non-interacting system are the same as those of the interacting one. One has to make informed guesses as to what this potential looks like. *(here we likely are on less solid ground:)*
- \Box But dealing with different numbers of particles, (A,Z) , including infinite, and not only at equilibrium density, one needs a way to generate this "mean field" in the same way for all these systems and densities
- ❑ Solution: I calculate it self-consistently from some in-medium effective interaction or effective Lagrangian. The guess work reduces to guessing the form of this interaction or Lagrangian.

"The energy is a function of the density"

The fundamental entity is the functional of the density; the effective interactions are auxiliary.

Skyrme effective interaction

$\hat{v}_{\rm Sk}(\mathbf{r}_{12}) = t_0 \left(1 + x_0 \hat{P}_{\sigma}\right) \delta(\mathbf{r}_{12}) + \frac{1}{2} t_1 \left(1 + x_1 \hat{P}_{\sigma}\right) \left[\hat{\mathbf{k}}^{\dagger 2} \delta(\mathbf{r}_1 + \delta(\mathbf{r}_{12}) \hat{\mathbf{k}}^2) + t_2 \left(1 + x_2 \hat{P}_{\sigma}\right) \hat{\mathbf{k}}^{\dagger} \cdot \delta(\mathbf{r}_{12}) \hat{\mathbf{k}}\right]$ $+\frac{1}{6}t_3(1+x_3\hat{P}_\sigma)\delta(\mathbf{r}_{12})\rho^{\alpha}(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}) +iW_0(\hat{\boldsymbol{\sigma}}_1+\hat{\boldsymbol{\sigma}}_2)\cdot\hat{\mathbf{k}}^{\dagger}\delta(\mathbf{r}_{12})\hat{\mathbf{k}}$

Skyrme energy per particle: density, asymmetry, gradients

$$
\mathcal{E}(\rho,\delta) = \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho + \frac{t_0}{8}(1+2x_0)\rho\delta^2 + \frac{t_3}{16}\rho^{1+\alpha} - \frac{t_3}{48}(1+2x_3)\rho^{1+\alpha}\delta^2
$$

$$
-\frac{1}{64}(3t_1 + 6t_1x_1 + t_2 + 2t_2x_2)\frac{(\nabla\rho\delta)^2}{\rho} + \frac{1}{64}(9t_1 - 5t_2 - 4t_2x_2)\frac{(\nabla\rho)^2}{\rho}
$$

50	symmetric matter	
t_0 : binding	$\frac{2}{5}$	20
$t_3\rho^\alpha$: saturation	$\frac{2}{5}$	30
$t_{1,2}$: kinetic	10	
$t_{1,2}$: kinetic	10	
$t_{2,3}$: kinetic	10	
$t_{3,3}$: kinetic	10	

 t_0 : binding

 $t_{1,2}$: kinetic

$$
+\frac{1}{8}(2t_1+t_1x_1+t_2+t_2x_2)\tau -\frac{1}{8}(t_1+2t_1x_1-t_2-2t_2x_2)\sum_{q=p,n}\frac{\rho_q\tau_q}{\rho} +\frac{1}{2}W_0(\frac{\mathbf{J}\cdot\nabla\rho}{\rho}+\sum_{q=p,n}\frac{\mathbf{J}_q\cdot\nabla\rho_q}{\rho}
$$

Skyrme mean field and restoring force for linear response (HF, RPA)

From functional differentiation of the above

❑ Now the EDF can mediate a learning process: from nuclei about nuclear matter and vice versa.

Characterization of the nuclear EoS

- The Taylor expansion coefficients of the energy per particle $E(\rho)$ at δ=0 around saturation density are conveniently used to characterize the nuclear EoS of isospin-symmetric nuclear matter.
- \Box The most relevant coefficients for nuclei are the saturation density ρ_0 itself, the energy at saturation density E_0 , the compression modulus K_0 , and the symmetry energy value J (cf. LDM).
- The first derivative at the saturation point vanishes by definition.

$$
E(\rho) = E_0 + \frac{1}{2} K_0 x^2 + \frac{1}{6} Q_0 x^3 + \dots
$$

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

❑ The symmetry energy also is characterized by a Taylor expansion,

$$
S(\rho) = J + Lx \frac{1}{2} K_{sym} x^2 + \frac{1}{6} Q_{sym} x^3 + ...
$$

Extrapolations beyond saturation are controlled by such parameters -20

density ffm⁻³1

Characterization of the nuclear EoS

Constraints on the EoS coefficients

- ❑ The most accessible nuclear properties are determined by the lower-order EoS coefficients and mostly by those for symmetric matter with the help of liquid drop models and energy density functional theory.
- ❑ As a result, the lower-order coefficients and those of symmetric matter are best determined $E_0 \approx -16$ MeV, $\rho_0 \approx 0.16$ fm⁻³, J \approx 30-33 MeV, ...
- Higher-order ones are important for extrapolations of the nucleonic EoS beyond saturation density
	- ⎯ Description of neutron star matter
	- Neutron skins
	- ⎯ Collective vibrations

Compression modulus $K_0 \approx 200$ -250 MeV, L ≈ 40 -70MeV, etc.

IRIS 중이온가속기연구소

See also: Roca-Maza&Paar, Prog.Part.Nucl.Phys. 101,96

Constraints on the EoS coefficients from collective excitations

Nuclear symmetry energy from various observables and calculations (examples)

Contents

02 Nuclear EDFT news

KIDS framework Correlation studies

Phenomenological energy-density functionals

Hundreds of EDF models for nuclei and nuclear matter

- ❑ Typically, ~ten parameters fitted to nuclear properties using different data sets and fitting protocols
- ❑ Very different predictions below and above saturation density
- ❑ Very different predictions at large isospin asymmetries

Phenomenological energy-density functionals

- ❑ Only few of the hundreds of EDF models can simultaneously describe nuclear matter and finite nuclei
- ❑ Spurious correlations among parameters have been noted; binding energies and seem to radii "prefer" different values for the effective mass

❑ Not a satisfactory situation at all:

"going from successful models in the description of observables to the EoS is a well defined and safe strategy while ensuring reasonable parameters of the EoS do not necessarily lead to a good reproduction of the data on finite nuclei."

□ Next: How we overcome these problems with **KIDS**

Dutra et al, PRC85(2012)035201 Stevenson et al., AIP Conf. Proc 1529.262

Bender et al., RMP75(2003)121

Roca-Maza&Paar, PPNP101(2018)96

KIDS **framework for the EoS and EDF**

KIDS: Korea, IBS,Daegu,SKKU G rown-ups: H. Gil, C.H.Hyun (Daegu Univ.) + P.P. (IBS) Past contributors: T.-S.Park, Y. Lim, Y. Oh, G. Ahn, Y.-M.Kim,J.Xu Currently collaborating: K.Yoshida, N.Hinohara

a Analytical form of EoS inspired by Brueckner and effective field theories: expansion in $k_F \sim \rho^{1/3}$

$$
\mathcal{E}(\rho,\delta) = \mathcal{T}(\rho,\delta) + \sum_{i=0}^{n} c_i(\delta)\rho^{1+i/3} \qquad \qquad \delta = (\rho_n - \rho_p)/\rho
$$

❑ In quadratic approximation:

$$
c_i(\delta) = \alpha_i + \beta_i \delta^2
$$
 and $S(\rho) = \sum_{i=0}^n \beta_i \rho^{1+i/3}$

❑ Straightforward analytical (linear) relations between standard EoS parameters and KIDS-EoS parameters; freedom to expand to as many EoS parameters as we wish

❑ **Can be readily transposed to an EDF without altering its parameters**

KIDS framework for the EoS and EDF

❑ Has the form of an extended Skyrme functional with generalized density dependence. First, we define a Skyrme-like effective interaction

$$
v_{ij} = (t_0 + y_0 P_\sigma) \delta(\mathbf{r}_i - \mathbf{r}_j)
$$

+ $\frac{1}{2} (t_1 + y_1 P_\sigma) [\delta(\mathbf{r}_i - \mathbf{r}_j) \mathbf{k}^2 + {\mathbf{k}'}^2 \delta(\mathbf{r}_i - \mathbf{r}_j)]$
+ $(t_2 + y_2 P_\sigma) \mathbf{k}' \cdot \delta(\mathbf{r}_i - \mathbf{r}_j) \mathbf{k}$
+ $\frac{1}{6} \sum_{n=1}^{N-1} (t_{3n} + y_{3n} P_\sigma) \rho^{n/3} \delta(\mathbf{r}_i - \mathbf{r}_j)$
+ $iW_0 \mathbf{k}' \times \delta(\mathbf{r}_i - \mathbf{r}_j) \mathbf{k} \cdot (\sigma_i - \sigma_j)$, notation:
instead of $t_i x_i$
we write y_i

❑ **Advantage: standard, efficient Skyrme-nuclear-structure codes can be used**

KIDS framework for the EoS and EDF

KIDS framework for the EoS and EDF

- ❑ Proof of principle: from the APR EoS straight to nuclei
- ❑ EoS parameters taken from fit of analytical KIDS form to APR
- ❑ Effective mass can be chosen and the results tested at will

Only fit gradient and spin-orbit terms to a few basic nuclear properties

Gil et al., Phys. Rev. C 99(2019)064319

Selected results from:

Xu&PP, Phys. Rev. C 105,044305 Zhou,Xu,PP, Phys. Rev. C 107, 055803 Gil et al., IJMPE 31, 2250013

- ❑ Bayesian analysis of nuclear properties; neutron-star properties
- ❑ Combined analyses of nuclear properties and neutron-star properties

Bayesian analysis of nuclear properties

Examined ²⁰⁸Pb and ¹²⁰Sn

Isovector constraints: Neutron skin thickness, giant dipole resonance, dipole polarizability

Isoscalar constraints: mass, charge radius, energy of the isoscalar monopole resonance Results for KIDS are compared with standard Skyrme-Hartree-Fock

Bayesian analysis of isoscalar nuclear properties

 -350 $1.0x10^{-2}$ -350 $1.0x10^{-2}$ (b) (a) 120 Sn $208Pb$ $8.0x10^{-3}$ $8.0x10^{-3}$ Q_0 (MeV)
 $\frac{1}{6}$ Q_0 (MeV)
 $\frac{1}{60}$ Skyrme: 6.0x10⁻³ $6.0x10^{-3}$ K_0 vs Q_0 $4.0x10^{-3}$ $4.0x10^{-3}$ $Eq.(3)$ $Eq.(3)$ $2.0x10^{-3}$ $2.0x10^{-3}$ -450 200 -450 200 $\overline{0.0}$ 0.0 210 220 230 240 210 220 230 240 K_0 (MeV) K_0 (MeV) 400 400 $1.0x10^{-4}$ $1.0x10⁻⁴$ (d) (C) 120 Sn $208Pb$ 8.0x10-5 8.0x10-5 KIDS : $\begin{array}{c}\nG_0 \text{ (MeV)} \\
\oplus \text{ (MeV)} \\
\oplus \text{ (MeV)}\n\end{array}$ $\overline{0}$ Q_{0} (MeV)
 \circ Ω $6.0x10^{-5}$ 6.0x10⁻⁵ Much broader PDFs $4.0x10^{-5}$ 4.0x10⁻⁵ (notice scale) $2.0x10^{-5}$ $2.0x10^{-5}$ -800 200 0.0 0.0 -800 230 240 210 230 240 210 220 220 200 K_0 (MeV) K_0 (MeV) Xu&PP, Phys. Rev. C 105,044305**IRIS 중이온가속기연구소**

Bayesian analysis of isoscalar nuclear properties

 -350 $1.0x10^{-2}$ -350 $1.0x10^{-2}$ (b) (a) 120 Sn $208Pb$ 8.0x10⁻³ $8.0x10^{-3}$ Q_0 (MeV)
 $\frac{1}{6}$ Q_0 (MeV)
 $\frac{1}{60}$ Skyrme: 6.0x10⁻³ $6.0x10^{-3}$ K_0 vs Q_0 $4.0x10^{-3}$ $4.0x10^{-3}$ $Eq.(3)$ $Eq.(3)$ $2.0x10^{-3}$ $2.0x10^{-3}$ -450 200 -450 200 $\overline{0.0}$ 0.0 210 220 230 240 210 220 230 240 K_0 (MeV) K_0 (MeV) 400 400 $1.0x10^{-4}$ $1.0x10⁻⁴$ (d) (C) 120 Sn $208Pb$ 8.0x10-5 8.0x10-5 KIDS : $\begin{array}{c}\nG_0 \text{ (MeV)} \\
\oplus \text{ (MeV)} \\
\oplus \text{ (MeV)}\n\end{array}$ $\overline{0}$ Q_{0} (MeV)
 \circ Ω $6.0x10^{-5}$ 6.0x10⁻⁵ Much broader PDFs $4.0x10^{-5}$ 4.0x10⁻⁵ (notice scale) $2.0x10^{-5}$ $2.0x10^{-5}$ -800 200 0.0 0.0 -800 230 240 210 230 240 210 220 220 200 K_0 (MeV) K_0 (MeV) Xu&PP, Phys. Rev. C 105,044305**IRIS 중이온가속기연구소**

Bayesian analysis of isoscalar nuclear properties

Bayesian analysis of isovector nuclear properties

120 $8.0x10^{-4}$ 120 $8.0x10^{-4}$ (h) (b) 100 100 6.4×10^{-4} $6.4x10⁻⁴$ (MeV) $\frac{L (M \text{eV})}{60}$ 80 4.8×10^{-4} $4.8x10^{-4}$ 60 Skyrme: 3.2×10^{-4} $3.2x10^4$ Ksym vs L 40 $1.6x10^{-4}$ $1.6x10⁴$ 20 20 120 Sn $208Pb$ 0.0 $-400 - 300 - 200 - 100 = 0$ 0.0 $-400 - 300 - 200 - 100 = 0$ 100 100 K_{sym} (MeV) K_{sym} (MeV) 120 $8x10^{-5}$ 120 $8x10^{-5}$ $\left(\mathsf{k}\right)$ (e) 100 100 $6x10^{-5}$ 6x10⁻⁵ (MeV) (MeV)
 $\frac{8}{8}$ KIDS : $5x10^{-5}$ $5x10^{-5}$ Broader PDFs $3x10^{-5}$ $3x10^{-5}$ ⊐ 40 Ksym not constrained $2x10^{-5}$ $2x10^{-5}$ 20 120 Sn 20 $208Pb$ Ω $-400 - 300 - 200 - 100 = 0$ $-400 - 300 - 200 - 100$ $\overline{0}$ 100 100 $\mathbf{0}$ K_{sym} (MeV) K_{sum} (MeV) Xu&PP, Phys. Rev. C 105,044305**IRIS 중이온가속기연구소**

Bayesian analysis of isovector nuclear properties

Xu&PP, Phys. Rev. C 105,044305

Bayesian analysis of isovector nuclear properties

Skyrme: *With line: shown*

*equation for representative ρ0, α, m**

KIDS : Broader PDFs Ksym unconstrained

Xu&PP, Phys. Rev. C 105,044305

Bayesian analysis of isovector nuclear properties

Skyrme:

*With line: shown equation for representative ρ0, α, m**

KIDS : Broader PDFs Ksym unconstrained

Xu&PP, Phys. Rev. C 105,044305

Bayesian analysis of isovector nuclear properties

Xu&PP, Phys. Rev. C 105,044305

Analyses of astronomical data Combined analysis with nuclear data

Corresponding EoS domains

KIDS model allows for

❑ Inflection point: soft-to-stiff transition,

important for description of dense matter

❑ Decoupling of dilute and dense regimes

 $208Pb$, J=33 MeV

Summary so far: J≈30-33 MeV, L ≈ 45-65 MeV, K_{sym} ≈ -150-0 MeV

Corresponding EoS domains

KIDS model allows for

❑ Inflection point: soft-to-stiff transition,

important for description of dense matter

❑ Decoupling of dilute and dense regimes

Summary so far: J≈30-33 MeV, L ≈ 45-65 MeV, K_{sym} ≈ -150-0 MeV

Contents

03 Recent developments

Density regimes Beyond one-body picture

- ❑ Distinct density domains in the EoS? (inspired by ongoing work on the PREXII, CREX, dipole polarizability puzzle)
- ❑ Beyond mean-field approaches: Fluffiness of Sn isotopes

Predictions for the neutron skin

RMF models

- ❑ KIDS predictions for the neutron skin when the parameters are constrained from gross nuclear properties (masses, charge radii) and neutron star properties, generally agree with CREX and underestimate $PREX$ – see C.H.Hyun, arXiv:2112.00996 *[~300 KIDS EDFs obeying EoS*] \Box The tension is similar to other studies, including
- Ir_{np;}(208_{Pb)} [fm] 0.2 0.18 0.16 0.14 2112.00996 [Phys.Rev.C103] 0.12 SLy4 0.1 0.1 0.14 0.18 0.22 0.26 Δr_{ND} (⁴⁸Ca) [fm]

CREX

0.26

 0.24

0.22

PREX-II

For a first study of CREX-PREX only, see arXiv:2210.02696 (Rila2022 proceedings)

What will it take to reconcile CREX, PREXII, a_n?

- ❑ Searching for KIDS parameter sets which reproduce both CREX and PREXII within their respective errors (1σ) and at the same time basic nuclear properties (<1%)
- Extend the formalism to vary freely up to 5+5 EoS parameters: including skewness and kyrtosis of both symmetric matter (Q $_{\rm 0}$, R $_{\rm 0}$) and symmetry energy (Q $_{\rm sym}$, R $_{\rm sym}$) , as follows:

 ρ_0 = 0.15-0.16 fm⁻³, E₀ = -16 MeV, K₀ = 200-240 MeV J = 30-36 MeV L = 40-70MeV

- K_{sym} varied widely in steps of 50 MeV
- Q_{0} , Q_{sym} varied widely in steps of 500MeV
- R_0 , R_{sym} varied widely in steps of 2 GeV

and in addition: C₁₂ = -66 MeV fm⁵, D₁₂ = 2.5 MeV fm⁵, m*/m = 0.82, κ = 0.22, W₀ = 133 MeV fm⁵

Results for a_D as well as neutron skin

Domain with best a_D

- ❑ Unorthodox but not necessarily unphysical behavior at low density
- ❑ Consistent with analyses of heavy-ion collisions

Domain with best a_p

- ❑ Unorthodox but not necessarily unphysical behavior at low density
- ❑ Consistent with analyses of heavy-ion collisions

Giant monopole resonance: Why is tin soft?

Garg&Colò, PPNP101(2018)55

- ❑ A description of the compression mode of Sn isotopes within self-consistent QRPA cannot be achieved at the same time as ²⁰⁸Pb and other previously studied nuclei; the energy is overestimated.
- ❑ In EoS terms, Sn isotopes require a lower model **compression modulus**: they are too "fluffy"

Giant monopole resonance: Why tin is soft

❑ QRPA+quasiparticle-vibration coupling based on relativistic functionals

v **RQRPA** Δ = 0.5 MeV Δ = 0.5 MeV **RQTBA** $S[10^3fm^4/MeV]$
 \sim \sim Exp 15 $\frac{-120}{5}$ Sn 1208 Pb (d) (c) $10¹$ $\boldsymbol{0}$ 20 25 15 15 10 20 10 5 25 5 E [MeV] E [MeV]

IRIS 중이온가속기연구소

Litvinova, PRC107(2023)L041302

Giant monopole resonance: Why tin is soft

❑ QRPA+quasiparticle-vibration coupling based on Skyrme HFB

Pondering the domain of orbital-based EDFT

- ❑ EDFT and self-consistent RPA as we know them are only expected to describe average singleparticle quantities; total sum rules. The detailed strength distribution is known to require beyondmean-field approaches, correlations, and the like.
- ❑ There is no self-consistent geminal-based (based on the two-particle density) response theory. Geminals are in use in quantum chemistry. There are advances for infinite nuclear matter based on the pair distribution function. Such may serve as guides.

Contents

Status summary

04 Conclusion

Progress in nuclear EDF

- ❑ Optimal number of EoS parameters eliminates spurious correlations btw parameters, observables We saw the examples of $\mathsf{K}_{\mathsf{sym}}$ vs J,L and of Q_{0} vs K_{0} .
- ❑ The effective mass not an impediment in EDFT: Static, bulk properties of nuclear systems are blind to the in-medium nucleon effective mass. *It may be important in dynamics of course
- ❑ The symmetry energy is predicted to have an inflection point which traditional functionals do not produce. It might be advisable to distinguish between the dilute and dense regimes.

Pondering the domain of orbital-based EDFT

❑ EDFT incl. self-consistent RPA are orbital-based and expected to describe average single-particle quantities, total sum rules. Detailed strength distributions are known to require beyond-mean-field approaches. Geminals can encode correlations and are in use in quantum chemistry. There are advances for infinite nuclear matter based on the pair distribution function. Such may serve as **IRIS 중이온가속기연구소** guides for approaches for nuclei.

Thank you!

대전광역시 유성구 국제과학로 1 1, Gukjegwahak-ro, Yuseong-gu, Daejeon, Korea

T 042 878 8827 ppapakon@ibs.re.kr

In conclusion

01 Nuclear EDFT

Droplet models:

Guessing the EDF form – part I: Brueckner theory

- ❑ Realistic potential: strong repulsive core plus attraction at longer range; apply Brueckner methodology in the calculation of nuclear matter energy
- □ Result: converging series of k_F^2 , k_F^3 , k_F^4 , ...
	- Even powers: from repulsive part
	- Odd powers: from both
- ❑ The relevant variable is *k^F* , or powers of *ρ 1/3*

Fetter&Walecka, Quantum theory of many-particle systems

Guessing the EDF form – part II: effective field theory

❑ Saturation density is low with respect to (effective) boson exchange range

One-pion exchange: vanishing expectation value

Next boson: rho with mass approx. 775 MeV or 4fm-1

Q Expansion of E/A in powers of k_F , which means again powers of $p^{1/3}$.

□ The k_F^3 and k_F^4 are known to be important for saturation

Natural Ansatz: E/A in powers of ρ Kaiser et al., NPA697(2002)255 **1/3**

Hammer&Furnstahl, NPA678(2000)277