

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

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01 Introduction

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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:)
- 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

$\hat{v}_{\text{Sk}}(\mathbf{r}_{12}) = t_0 (1 + x_0 \hat{P}_{\sigma}) \,\delta(\mathbf{r}_{12}) + \frac{1}{2} t_1 (1 + x_1 \hat{P}_{\sigma}) [\hat{\mathbf{k}}^{\dagger 2} \delta(\mathbf{r}_1 + \delta(\mathbf{r}_{12}) \hat{\mathbf{k}}^2] + t_2 (1 + x_2 \hat{P}_{\sigma}) \,\hat{\mathbf{k}}^{\dagger} \cdot \delta(\mathbf{r}_{12}) \hat{\mathbf{k}}$ $+ \frac{1}{6} t_3 \left(1 + x_3 \hat{P}_{\sigma}\right) \,\delta(\mathbf{r}_{12}) \rho^{\alpha} \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right) + i W_0 \left(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2\right) \cdot \hat{\mathbf{k}}^{\dagger} \,\delta(\mathbf{r}_{12}) \hat{\mathbf{k}}$

Skyrme energy per particle: density, asymmetry, gradients

$$\mathcal{E}(\rho,\delta) = \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho + \frac{t_0}{8}(1+2x_0)\rho\delta^2 + \frac{t_3}{16}\rho^{1+\alpha} - \frac{t_3}{48}(1+2x_3)\rho^{1+\alpha}\delta^2 - \frac{1}{64}(3t_1+6t_1x_1+t_2+2t_2x_2)\frac{(\nabla\rho\delta)^2}{\rho} + \frac{1}{64}(9t_1-5t_2-4t_2x_2)\frac{(\nabla\rho)^2}{\rho}$$

$$t_0: binding$$

 $t_3 p^{\alpha}: saturation$
 $t_{1,2}: kinetic$

 $t_{\beta}\rho^{\alpha}$: sati

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

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 $\delta=0$ around saturation density are conveniently used to characterize the nuclear EoS of isospin-symmetric nuclear matter.
- The most relevant coefficients for nuclei are the saturation density ρ₀ itself, the energy at saturation density E₀, the compression modulus K₀, and the symmetry energy value J (cf. LDM).
- □ The first derivative at the saturation point vanishes by definition.

$$\Xi(\rho) = E_0 + \frac{1}{2} K_0 x^2 + \frac{1}{6} Q_0 x^3 + \dots$$
$$x = (\rho - \rho_0) / 3\rho_0$$

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





turation density

matter.

All these parameters have simple analytical

forms in the Skyrme

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Extrapolations beyond saturation are controlled by such parameters -20





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 $E_0 \approx -16 \text{ MeV}$, $\rho_0 \approx 0.16 \text{ fm}^{-3}$, J ≈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.

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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)



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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 **%**708

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

MDS framework for the EoS and EDF

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

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

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

□ 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

$$\begin{split} v_{ij} &= (t_0 + y_0 P_\sigma) \delta(\mathbf{r}_i - \mathbf{r}_j) \\ &+ \frac{1}{2} (t_1 + y_1 P_\sigma) [\delta(\mathbf{r}_i - \mathbf{r}_j) \mathbf{k}^2 + \mathbf{k'}^2 \delta(\mathbf{r}_i - \mathbf{r}_j)] \\ &+ (t_2 + y_2 P_\sigma) \mathbf{k'} \cdot \delta(\mathbf{r}_i - \mathbf{r}_j) \mathbf{k} \\ &+ \frac{1}{6} \sum_{n=1}^{N-1} (t_{3n} + y_{3n} P_\sigma) \rho^{n/3} \delta(\mathbf{r}_i - \mathbf{r}_j) \\ &+ i W_0 \, \mathbf{k'} \times \delta(\mathbf{r}_i - \mathbf{r}_j) \, \mathbf{k} \cdot (\sigma_i - \sigma_j), \end{split} \qquad \begin{array}{c} \text{notation:} \\ \text{instead of } t_i x_i \\ \text{we write } y_i \end{array}$$

□ 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

⁴⁰Ca9 90Zr 160 208ph 132Sn 8 E/A [MeV] ⁶⁰Ca 218 7 ²⁸0 6 ²⁰⁸Pb 👴 218 132Sn R_c [fm] ⁴⁰Ca • • 60Ca K0=240 MeV 3 16O 280 0.6 ⁶⁰Ca Δr_{np} [fm] 0.4 132Sn 208pb 0.2 4802 218 40Ca 0 160 40 80 120 160 200

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

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Mass number A



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

	Δr_{np} (fm)	E_{-1} (MeV)	$\alpha_D ~(\mathrm{fm}^3)$
²⁰⁸ Pb	0.283 ± 0.071	13.46 ± 0.10	19.6 ± 0.6
¹²⁰ Sn	0.150 ± 0.017	15.38 ± 0.10	8.59 ± 0.37

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 -350 1.0x10⁻² 1.0x10⁻² (b) (a)¹²⁰Sn ²⁰⁸Pb 8.0x10⁻³ 8.0x10⁻³ (MeV) 00-400 (MeV) 00. Skyrme: 6.0x10⁻³ 6.0x10⁻³ Ko vs Qo 4.0x10⁻³ 4.0x10⁻³ Eq.(3) Eq.(3) 2.0x10⁻³ 2.0x10⁻³ -450 -200 -450 0.0 0.0 ²²⁰ K₀ (MeV) 210 220 230 240 210 230 240 K_o (MeV) 400 400 1.0x10⁻⁴ 1.0x10⁻⁴ (d) (C) ¹²⁰Sn 208 Pb 8.0x10⁻⁵ 8.0x10⁻⁵ **KIDS** : 0 00-400 0 0 00-400 0 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_o (MeV) K_o (MeV) Xu&PP, Phys. Rev. C 105,044305 RIS 중이온가속기연구소

Bayesian analysis of isoscalar nuclear properties

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Bayesian analysis of isoscalar nuclear properties



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Bayesian analysis of isovector nuclear properties

8.0x10⁻⁴ 120 8.0x10⁻⁴ (h)(b) 100 100 6.4x10⁻⁴ 6.4x10⁻⁴ (Nev) 80 (NeV) 1 4.8x10-4 4.8x10⁻⁴ 60 Skyrme: 3.2x10⁻⁴ 3.2x10⁻⁴ 40 Ksym vs L 1.6x10⁻⁴ 1.6x10⁻⁴ 20 20 ¹²⁰Sn ²⁰⁸Pb 0.0 -400 -300 -200 -100 0 0.0 -400 -300 -200 -100 0 100 100 K_{svm} (MeV) K_{sym} (MeV) 120 120 8x10-5 8x10⁻⁵ (k) (e) 100 100 6x10⁻⁵ 6x10-5 (MeV) 90 **KIDS** : (MeV) 00 5x10-5 5x10⁻⁵ **Broader PDFs** 3x10-5 3x10-5 _ 40 K_{svm} not constrained 2x10-5 2x10⁻⁵ 20 120 Sn 20 ²⁰⁸Pb 0 -400 -300 -200 -100 0 0 -400 -300 -200 -100 100 100 0 K_{sym} (MeV) K_{svm} (MeV)

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

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 ρ_0, α, m^*

۲۵۵ : Broader PDFs K_{sym} unconstrained



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



Bayesian analysis of isovector nuclear properties



Skyrme:

With line: shown equation for representative ρ_0, α, m^*

۲۵۵ : Broader PDFs K_{sym} unconstrained



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

Bayesian analysis of isovector nuclear properties





Analyses of astronomical data

$R_{1.4}$ (km) $R_{2.08}$ (km) $\Lambda_{1.4}$ M_{max} c_s	$11.725 \pm 1.105 [15]$ $13.7^{+2.6}_{-1.5} [13] \text{ and } 12.39^{+1}_{-0}$ $190^{+390}_{-120} [18]$ $> 2.08M_{\odot} [12]$ < 1] ³⁰ ₉₈ [14]
150 () () () () () () () () () () () () ()	KIDS 0.01 posterior 0.01 0.00 0.00	 5 2 9 6
30 O Zhou,Xu,PP, Phys. Rev. C 107,	$ \begin{array}{c} (h) = 0.00 \\ & (h) = 0.00 \\ 1 & 2 & 3 \\ \rho/\rho_0 \\ 055803 \end{array} $	3 0 IRIS 중이온가속기연구소

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

80 KIDS SHF 70 60 energy [MeV] 50 40 30 20 10 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0 density [fm⁻³]

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



²⁰⁸Pb, J=33 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 \approx 30-33 MeV, L \approx 45-65 MeV, K_{sym} \approx -150-0 MeV



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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

- 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]
 The tension is similar to other studies, including
- The tension is similar to other studies, including RMF models





For a first study of CREX-PREX only, see

arXiv:2210.02696 (Rila 2022 proceedings)

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

- 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%)</p>
- Extend the formalism to vary freely up to 5+5 EoS parameters: including skewness and kyrtosis of both symmetric matter (Q₀, R₀) and symmetry energy (Q_{sym}, R_{sym}), as follows:

 $\rho_0 = 0.15 - 0.16 \text{ fm}^{-3}$, $E_0 = -16 \text{ MeV}$, $K_0 = 200 - 240 \text{ MeV}$ J = 30-36 MeV L = 40-70 MeV

- 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: $C_{12} = -66 \text{ MeV fm}^5$, $D_{12} = 2.5 \text{ MeV fm}^5$, $m^*/m = 0.82$, $\kappa = 0.22$, $W_0 = 133 \text{ MeV fm}^5$



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_D

- □ 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



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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.

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04 Conclusion

Progress in nuclear EDF

- Optimal number of EoS parameters eliminates spurious correlations btw parameters, observables
 We saw the examples of K_{svm} vs J,L and of Q₀ vs K₀.
- 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 guides for approaches for nuclei.

Thank you!



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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
- **Q** 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 $\rho^{1/3}$

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
- $\hfill\square$ Expansion of E/A in powers of k_F , which means again powers of $\rho^{1/3}$.
- □ The k_{F^3} and k_{F^4} are known to be important for saturation

Natural Ansatz: E/A in powers of $\rho^{1/3}$

Hammer&Furnstahl, NPA678(2000)277 Kaiser et al., NPA697(2002)255