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LEA COLLIGA MEETING

Beyond mean-field models with zero-range effective interactions: A way too handle the ultraviolet divergence

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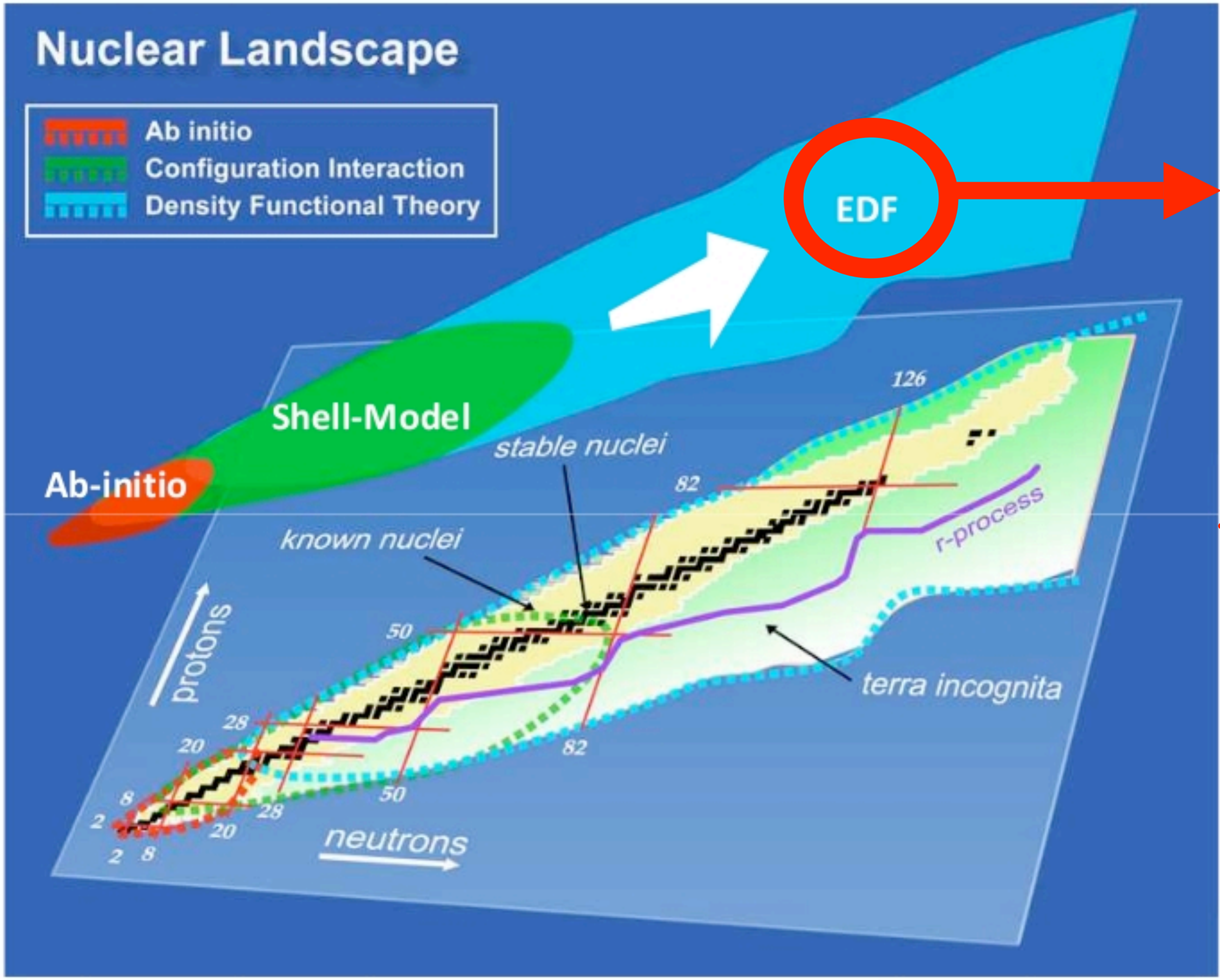
Milano-Orsay collaboration

- PhD thesis K. Moghrabi, Orsay
- Moghrabi, Grasso, Colò, Van Giai, *Beyond Mean-Field Theories with Zero-Range Effective Interactions: A Way to Handle the Ultraviolet Divergence*, PRL 105, 262501 (2010)
- Moghrabi, Grasso, Roca-Maza, Colò, *Second-order equation of state with the full Skyrme interaction: toward new effective interactions for beyond mean-field models*, in preparation
- 3 months visitor in IPN Orsay, Marco Brenna. *Particle-vibration coupling models: starting applications to nuclei*

A unified theory for nuclear structure, reactions and stars

The Energy Density Functional (EDF) Concept



http://unedf.org/

- ***Mean field for ground-state nuclear structure (HF, HFB,..)***
- ***RPA and QRPA for small-amplitude oscillations***
- ***Beyond small-amplitude oscillations: time-dependent mean field for dynamics (TDHF, TDHFB,…)***
- ***Beyond-mean - field models (correlations).***

  - Describing complex phenomena

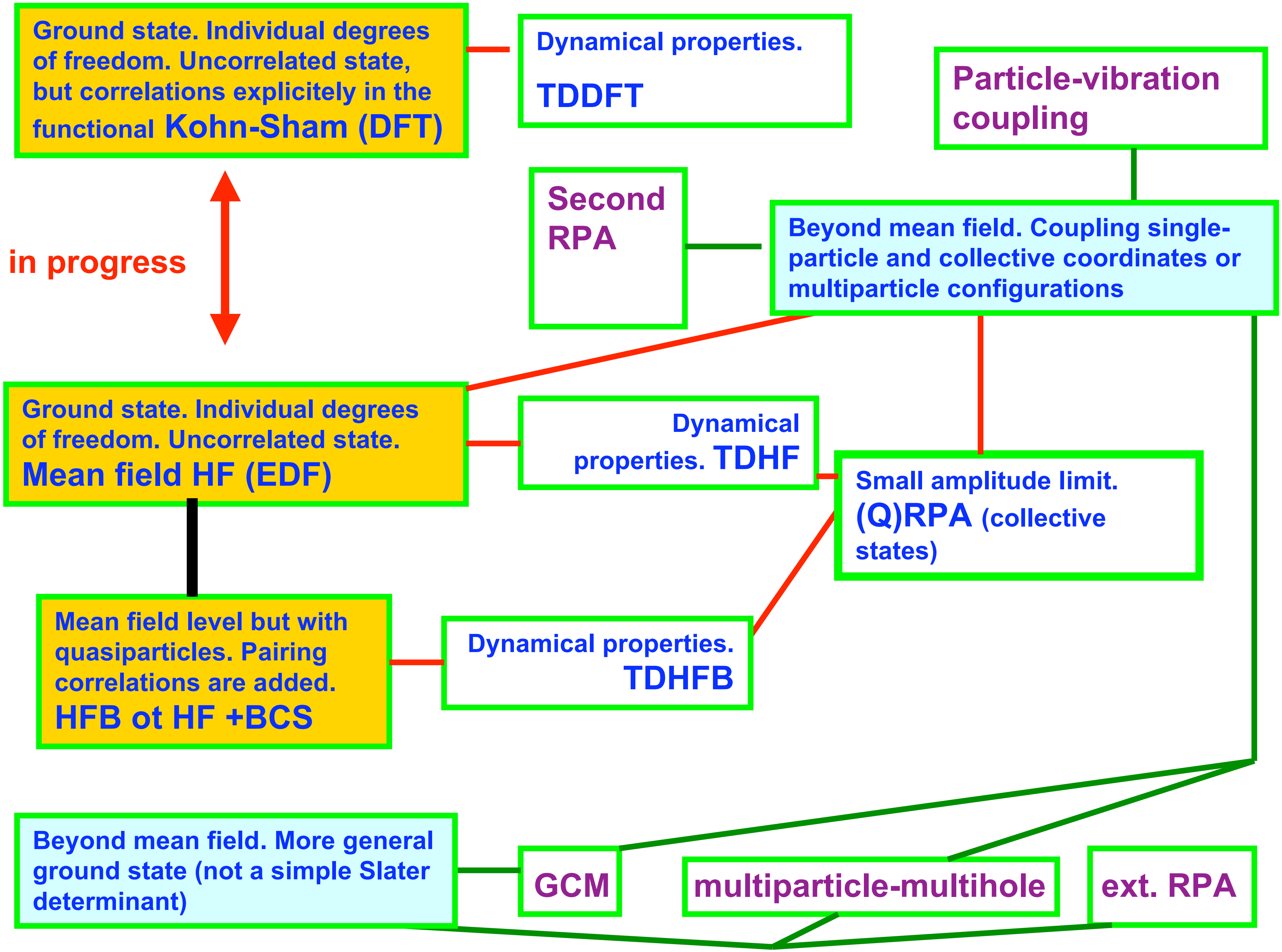
  - Improving the predictive power

Beyond-mean-field models. Some examples

- **Single-particle and collective degrees of freedom are coupled** (generator-coordinate method, particle-vibration coupling,…)

- **Single-particle and multi-particle degrees of freedom are coupled** (variational multiparticle-multihole configuration mixing, second RPA,…)

- **Correlations are explicitly included in the ground state** (extensions of RPA and SRPA, generator-coordinate method, variational multiparticle-multihole configuration mixing,…)


Ground state. Individual degrees of freedom. Uncorrelated state, but correlations explicitely in the functional Kohn-Sham (DFT)
Dynamical properties.
TDDFT
Particle-vibration coupling
in progress
Second RPA
Beyond mean field. Coupling single-particle and collective coordinates or multiparticle configurations
Ground state. Individual degrees of freedom. Uncorrelated state.
Mean field HF (EDF)
Dynamical properties. TDHF
Small amplitude limit.
(Q)RPA (collective states)
Mean field level but with quasiparticles. Pairing correlations are added.
HFB ot HF +BCS
Dynamical properties.
TDHFB
Beyond mean field. More general ground state (not a simple Slater determinant)
GCM
multiparticle-multihole
ext. RPA

How to handle beyond-mean-field theories: two issues

Nuclear physics: phenomenological effective interactions adjusted at the mean-field level ***(double counting?)***

When the interaction has zero range -> ***ultraviolet divergence*** **in some cases**

Some examples:

- *Pairing with a zero-range interaction (within the mean-field approximation)*

- *Models with particle-vibration coupling (see talk of Marco Brenna)*

- *Second RPA (see talk of Danilo Gambacurta)*

Some solutions:

- Pairing with a zero-range interaction (within the mean-field approximation)

Add and substract a quantity easy to handle which has the same divergent behavior as the divergent quantity of the theory. Pseudopontential method to extract the regulated part.

- Bruun, Castin, Dum, Burnett, Eur. Phys. J. D 7, 433 (1999)

- Grasso, Urban, PRA 68, 033610 (2003)

- Bulgac, Yu, PRL 88, 042504 (2002)

Grasso, Urban, PRA 68, 033610 (2003)

$$\Delta(\boldsymbol{R}) = -g \lim_{r\to 0} \frac{\partial}{\partial r}\left[r \left\langle \Psi_\uparrow\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)\Psi_\downarrow\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)\right\rangle\right].$$

g is the coupling constant of the delta interaction.

Pseudopotential prescription (for a quantity that diverges as 1/r for r->0)

The anomalous density diverges with a zero-range pairing interaction

Grasso, Urban, PRA 68, 033610 (2003)

g is the coupling constant of the delta interaction.

$$\Delta(\boldsymbol{R}) = -g \lim_{r\to 0} \frac{\partial}{\partial r}\left[r \left\langle \Psi_\uparrow\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)\Psi_\downarrow\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)\right\rangle \right]. \quad (8)$$

In practice, Eq. (8) is evaluated as follows: It is possible to show that the expectation value $\langle \Psi_\uparrow(\boldsymbol{R}+\boldsymbol{r}/2)\Psi_\downarrow(\boldsymbol{R}-\boldsymbol{r}/2)\rangle$ diverges as $\Delta/(4\pi r)$ when $r\to 0$ if a zero-range interaction is used. Now one adds and subtracts from this expectation value the quantity $\frac{1}{2}\Delta(\boldsymbol{R})G^0_\mu(\boldsymbol{R},\boldsymbol{r})$, where G^0_μ is Green's function associated to the single-particle Hamiltonian H_0,

$$G^0_\mu(\boldsymbol{R},\boldsymbol{r}) = \sum_\alpha \frac{\phi^0_\alpha\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right)\phi^{0*}_\alpha\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right)}{\epsilon^0_\alpha - \mu},$$

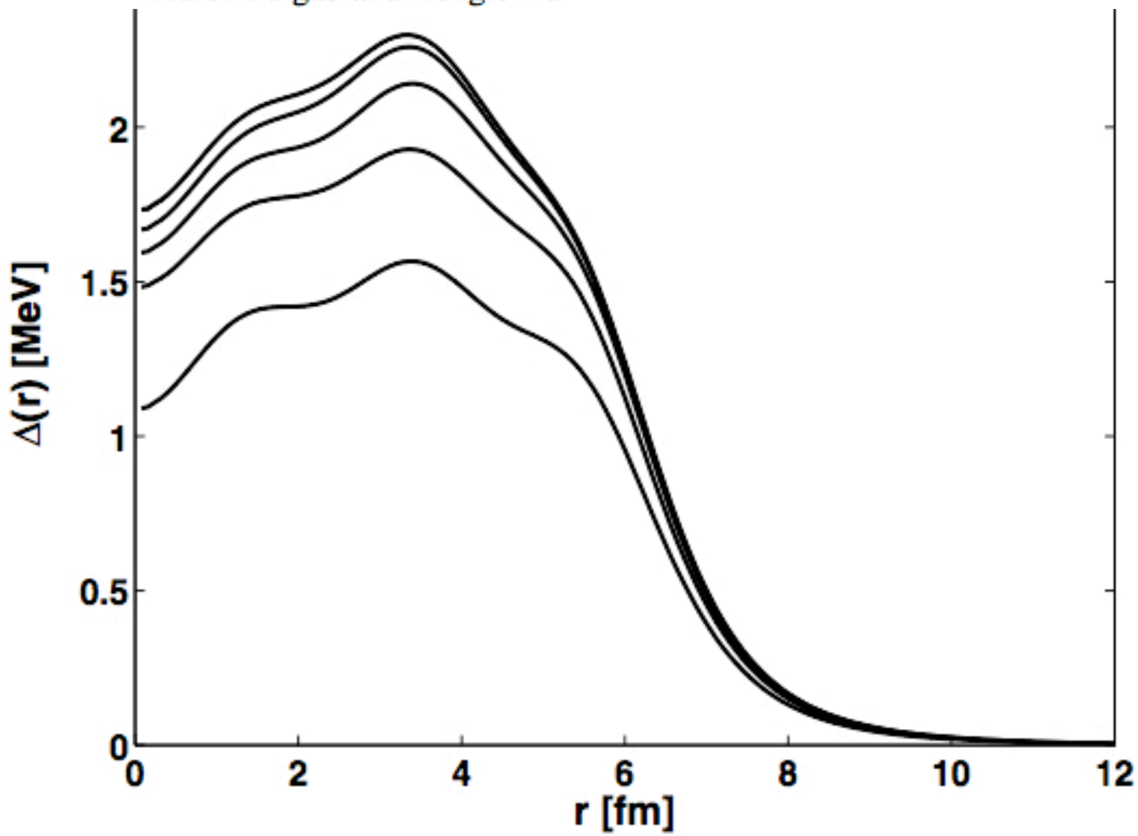
Diverges as $1/(2\pi r)$ when $r\to 0$

where ϕ^0_α denotes the eigenfunction of H_0 with eigenvalue $\epsilon^0_\alpha - \mu$.

Renormalization of the Hartree-Fock-Bogoliubov Equations in the Case of a Zero Range Pairing Interaction

Aurel Bulgac and Yongle Yu

HFB calculation done with a Woods-Saxon potential with fixed parameters corresponding to the nucleus ^{110}Sn and with a zero-range pairing force



The neutron pairing field (17) as a function of the radial coordinate and the cutoff energy E_c. Upward various curves correspond to $E_c = 20, 30, 35, 40, 45$, and 50 MeV, respectively. On the scale of the figure the last two curves are indistinguishable.

Beyond mean-field theories with zero-range effective interactions. How to handle the ultraviolet divergence at second order ?

Beyond Mean-Field Theories with Zero-Range Effective Interactions: A Way to Handle the Ultraviolet Divergence

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Zero-range effective interactions are commonly used in nuclear physics and in other domains to describe many-body systems within the mean-field model. If they are used within a beyond-mean-field framework, contributions to the total energy that display an ultraviolet divergence are found. We propose a general strategy to regularize this divergence and we illustrate it in the case of the second-order corrections to the equation of state (EOS) of uniform symmetric matter. By setting a momentum cutoff Λ, we show that for every (physically meaningful) value of Λ it is possible to determine a new interaction such that the EOS with the second-order corrections reproduces the empirical EOS, with a fit of the same quality as that obtained at the mean-field level.

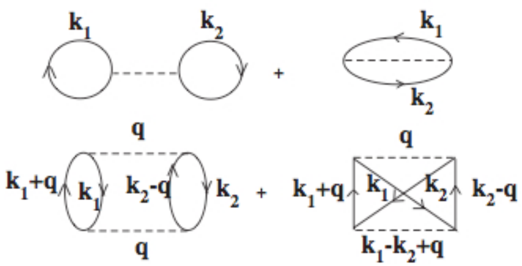


FIG. 1. First- and second-order diagrams for the total energy in uniform matter. Labels refer to momentum states.

… with a momentum cutoff

In the case of effective interactions between point-nucleons, the cutoff Λ must certainly be smaller than the momentum associated with the nucleon size, i.e., smaller than ≈ 2 fm^{-1}. In fact, these interactions are used to describe giant resonances or rotational bands of nuclei and consequently the scale should be even smaller, perhaps around 0.5 fm^{-1}. However, our procedure is tailored on the

Skyrme interaction

$$V(\mathbf{r}_1, \mathbf{r}_2) =$$

$$t_0 (1 + x_0 P_\sigma) \delta(\mathbf{r}) \quad \text{terme central}$$

$$+\frac{1}{2} t_1 (1 + x_1 P_\sigma) \left[\mathbf{P}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{P}^2 \right] + t_2 (1 + x_2 P_\sigma) \, \mathbf{P}' \cdot \delta(\mathbf{r}) \mathbf{P} \quad \text{termes non-locaux}$$

$$+\frac{1}{6} t_3 (1 + x_3 P_\sigma) [\rho(\mathbf{R})]^\alpha \delta(\mathbf{r}) \quad \text{terme dépendant de la densité}$$

$$+\mathrm{i} W_0 \, \boldsymbol{\sigma} \cdot \left[\mathbf{P}' \times \delta(\mathbf{r}) \mathbf{P} \right] \quad \text{terme spin-orbite}$$

Let us write the zero-range force as

$$V(\mathbf{r}_1, \mathbf{r}_2) = g\delta(\mathbf{r}_1 - \mathbf{r}_2).$$

To make contact with the Skyrme interactions [1] the strength g is written as $\boxed{t_0 + \frac{1}{6}t_3\rho^\alpha}$ and this corresponds to the so-called (t_0, t_3) model

Symmetric nuclear matter; t_0-t_3 model

Mean field

$$\frac{E}{A}(\rho) = \frac{3\hbar^2}{10m}\left(\frac{3\pi^2}{2}\rho\right)^{2/3} + \frac{3}{8}t_0\rho + \frac{1}{16}t_3\rho^{\alpha+1}.$$

Second-order correction

$$\Delta E = d\frac{\Omega^3}{(2\pi)^9}\int_{k_1,k_2<k_F,|\mathbf{k}_1+\mathbf{q}|,\mathbf{k}_2-\mathbf{q}|>k_F} \times d^3k_1 d^3k_2 d^3q \frac{v^2}{\epsilon_{\mathbf{k}_1} + \epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_1+\mathbf{q}} - \epsilon_{\mathbf{k}_2-\mathbf{q}}} \equiv C\int dq v^2 G(q),$$

d=$(n^2$-n)/2, n being the level of degeneracy (4 for symmetric nuclear matter)

Corrected equation of state. Linear divergence in the momentum cutoff

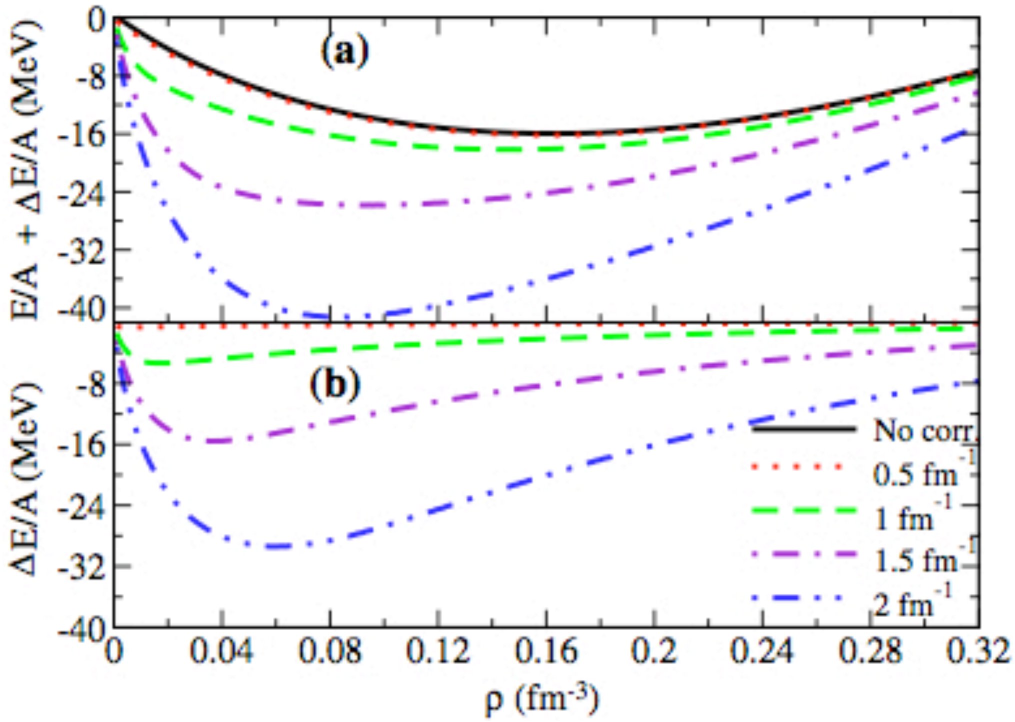


FIG. 2 (color online). (a) $E/A + \Delta E/A$ as a function of the density and for different values of the cutoff Λ. The SkP mean-field EOS (solid black line) is shown for comparison. (b) Correction $\Delta E/A$ for different values of Λ.

Moghrabi, Grasso, Colò, Van Giai, Phys. Rev. Lett. 105, 262501 (2010)

Equation of state after the fit

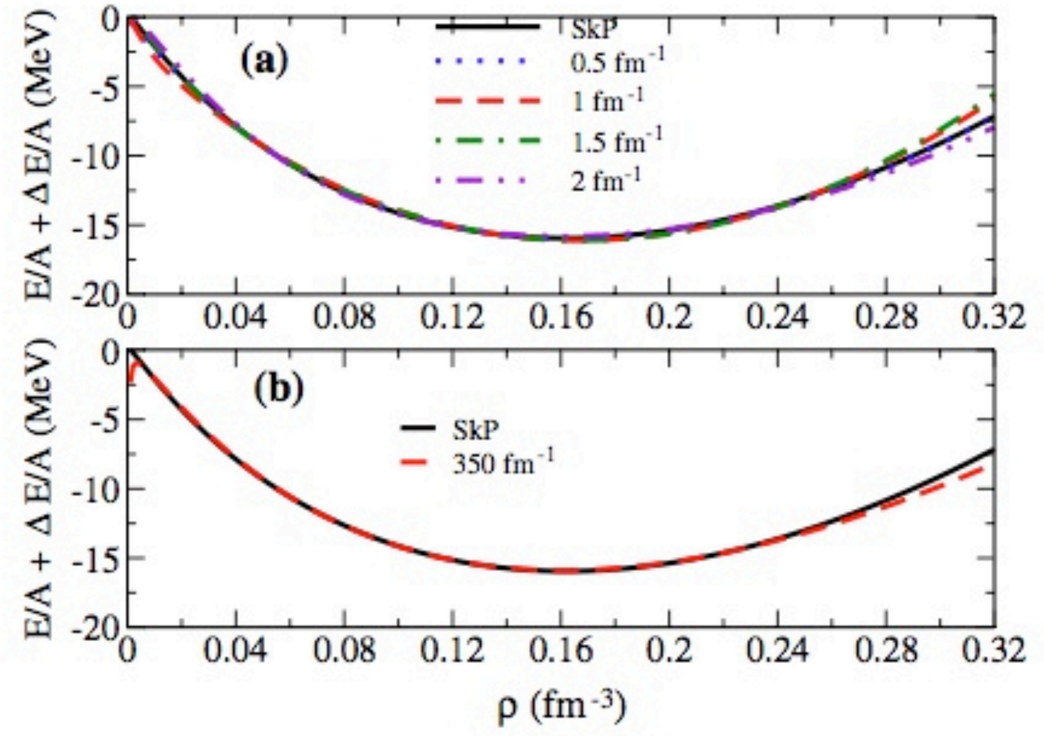


FIG. 4 (color online). (a) Second-order-corrected equations of state compared with the reference equation of state (SkP at mean-field level). (b) Extreme case of $\Lambda = 350\ \mathrm{fm}^{-1}$.

Moghrabi, Grasso, Colò, Van Giai, Phys. Rev. Lett. 105, 262501 (2010)

New parameters for each cutoff

TABLE I. From the second line, columns 2, 3, and 4: parameter sets obtained in the fits associated with different values of the cutoff Λ compared with the original set SkP (first line). In the fifth column the χ^2/N value (χ^2 divided by the number of fitted points) associated to each fit is shown. In columns 6 and 7 the saturation point is shown.

	t_0 (MeV fm^3)	t_3 (MeV fm$^{3+3\alpha}$)	α	χ^2/N	ρ_0 (fm^{-3})	$E/A(\rho_0)$ (MeV)
SkP	−2931.70	18 708.97	1/6		0.16	−15.95
$\Lambda = 0.5$ fm^{-1}	−2352.900	15 379.861	0.217	0.000 04	0.16	−15.96
$\Lambda = 1$ fm^{-1}	−1155.580	9435.246	0.572	0.001 42	0.17	−16.11
$\Lambda = 1.5$ fm^{-1}	−754.131	8278.251	1.011	0.001 06	0.17	−16.09
$\Lambda = 2$ fm^{-1}	−632.653	5324.848	0.886	0.001 92	0.16	−15.82
$\Lambda = 350$ fm^{-1}	−64.904	360.039	0.425	0.000 42	0.16	−15.88

Moghrabi, Grasso, Colò, Van Giai, Phys. Rev. Lett. 105, 262501 (2010)

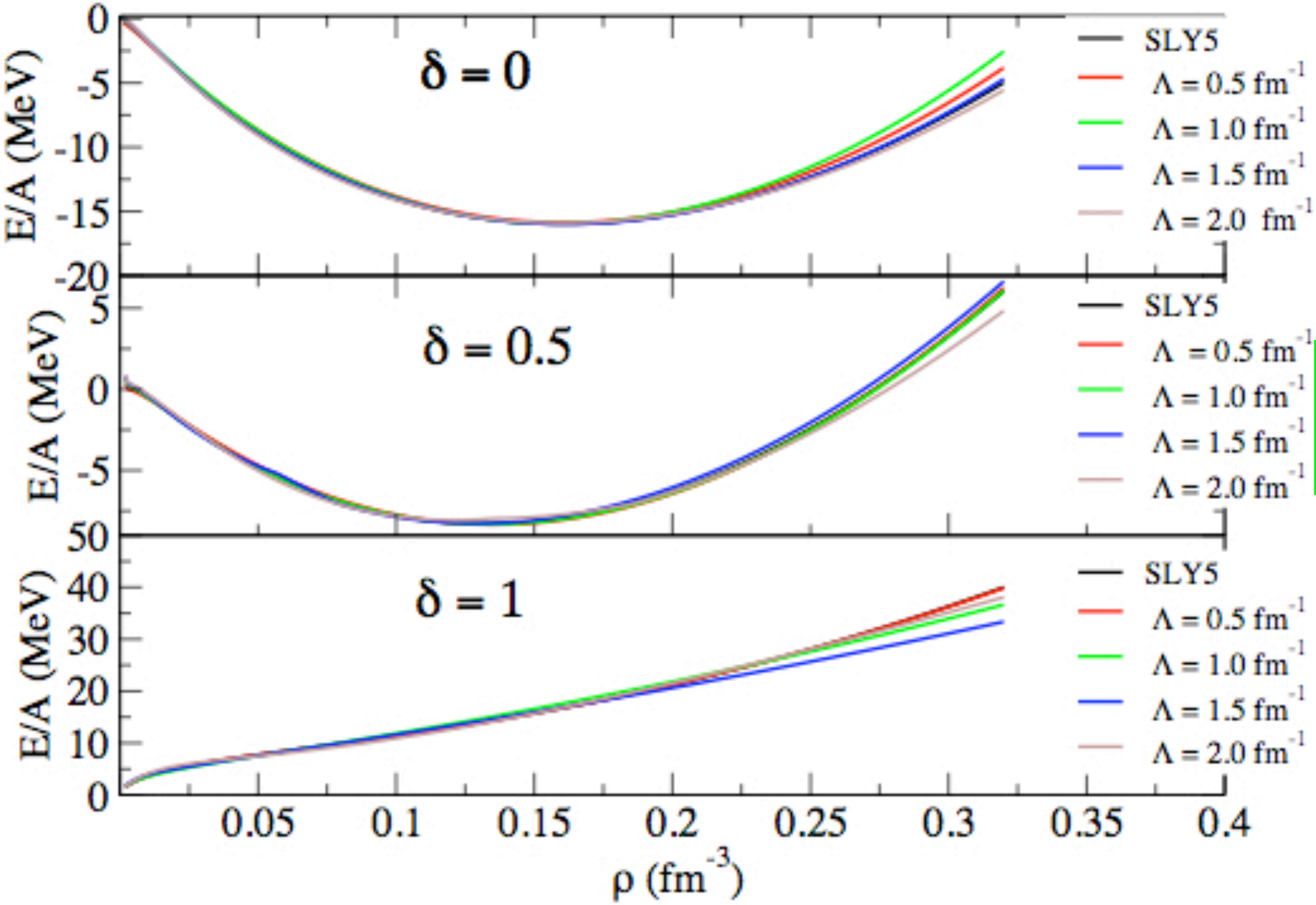
Extended case. The full Skyrme interaction and both symmetric and asymmetric matter

* Analytical study: the divergence is now Λ^5 due to the velocity-dependent terms of the interaction

* Cutoff regularization for both symmetric and asymmetric matter

* Adjustment of parameters (reference EOS: Sly5)

Three equations of state

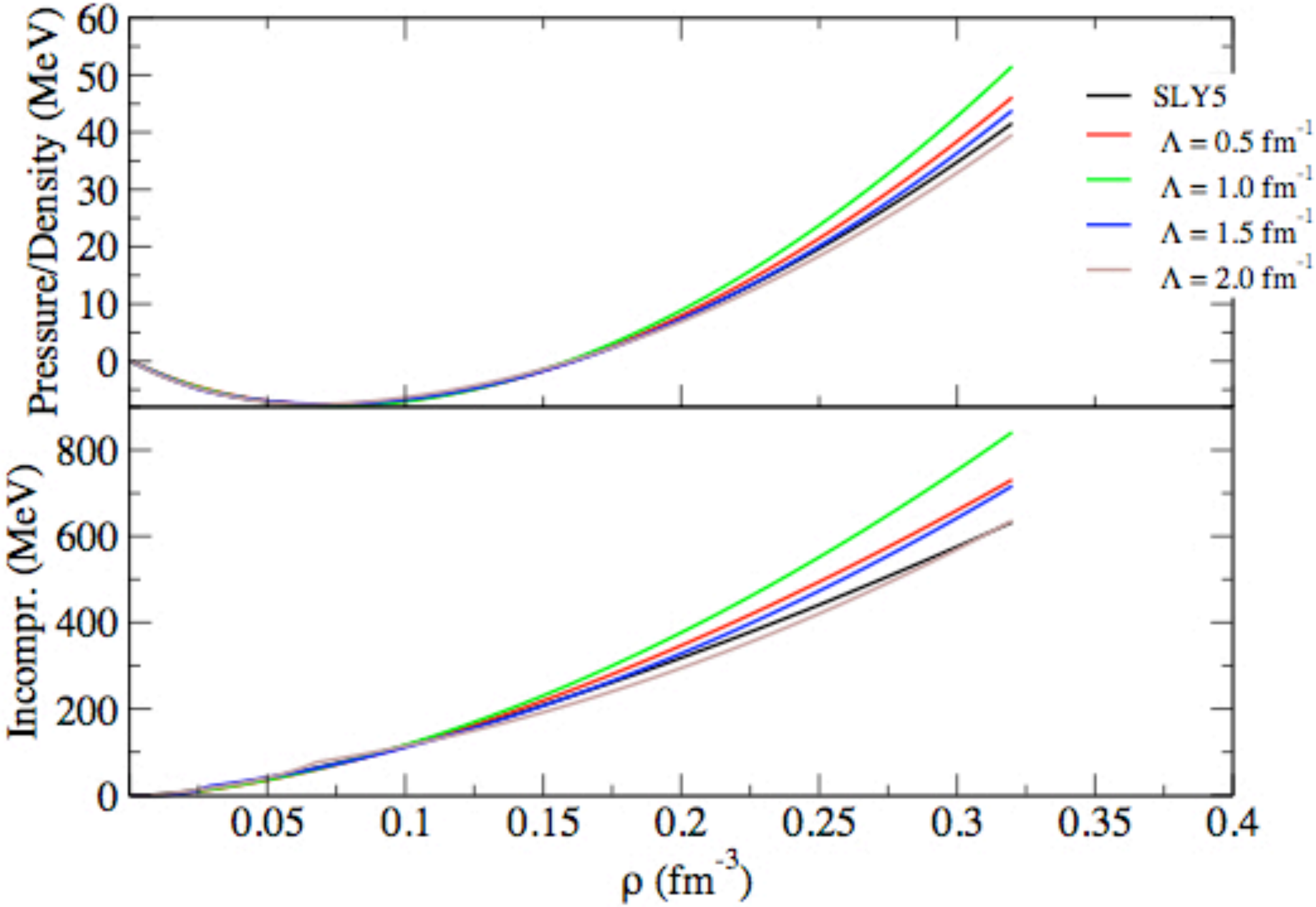


Symmetric matter

Asymmetric matter

Neutron matter

Pressure/density and incompressibility



Sets of parameters for each cutoff

	t_0	t_1	t_2	t_3	x_0	x_1	x_2	x_3	α
SLy5	-2484.88	483.13	-549.40	13736.0	0.778	-0.328	-1.0	1.267	0.16667
$\Lambda(\mathrm{fm}^{-1})$									
0.5	-2782.829	473.127	269.686	13322.999	0.897	-0.327	-1.005	1.379	0.0989
1.0	-2554.419	758.941	248.433	9331.697	0.852	0.811	-0.900	0.971	0.0111
1.5	-779.936	1127.769	-941.203	4428.398	1.135	0.119	-0.568	-0.403	0.813
2.0	-585.187	579.808	-596.216	4903.544	0.973	-0.323	-0.662	1.780	0.9002

Perspectives

- **Other renormalization procedures (dimensional renormalization -> <u>unique set of parameters</u>)**

- **Applications to finite nuclei**

- **Particle-vibration coupling models (formal and numerical work)**

- **… other beyond-mean-field theories?**