2019年度 原子核三者若手夏の学校

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Nuclear density functional theory: From fundamentals to frontiers

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Contents

Fundamentals of Density Functional Theory

- Interesting viewpoints on **DFT**
- Hohenberg-Kohn (**HK**) theorem
- Kohn-Sham (**KS**) scheme
- *Discussion*: some open issues

Nuclear DFT and applications

- Covariant Density Functional Theory (**CDFT**)
- *Application*: Nuclear tensor force and its effects

Connections to Quantum Field Theory

- Energy density functional and effective action in **QFT**
- Functional Renormalization Group (**FRG**)
- *Application*: φ^4-theory in zero dimension

Nuclear chart

stable nuclei ~ 300 nuclei

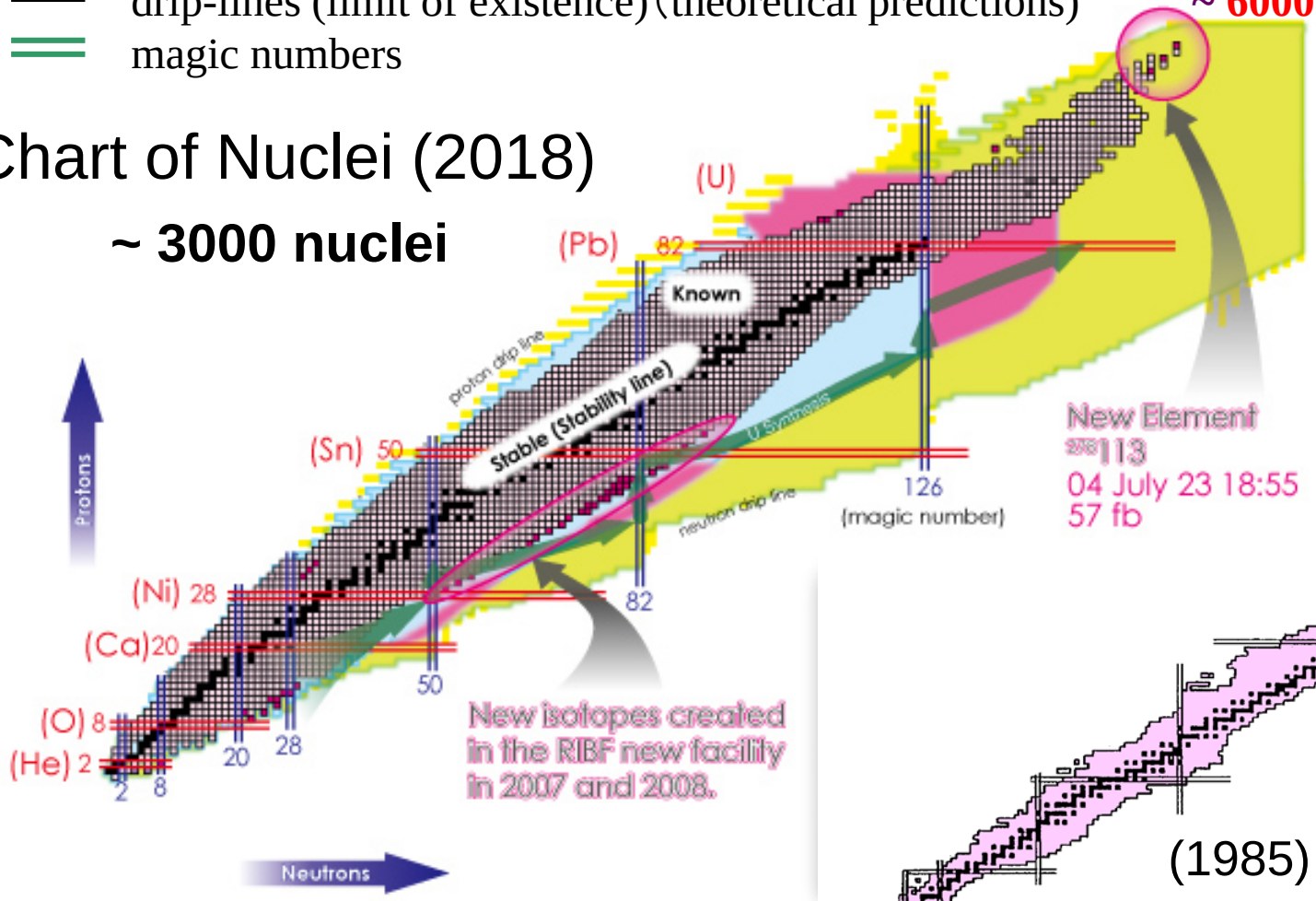
unstable nuclei observed so far ~ 3000 nuclei

drip-lines (limit of existence)（theoretical predictions) ~ 6000 nuclei

magic numbers

Chart of Nuclei (2018)

~ 3000 nuclei

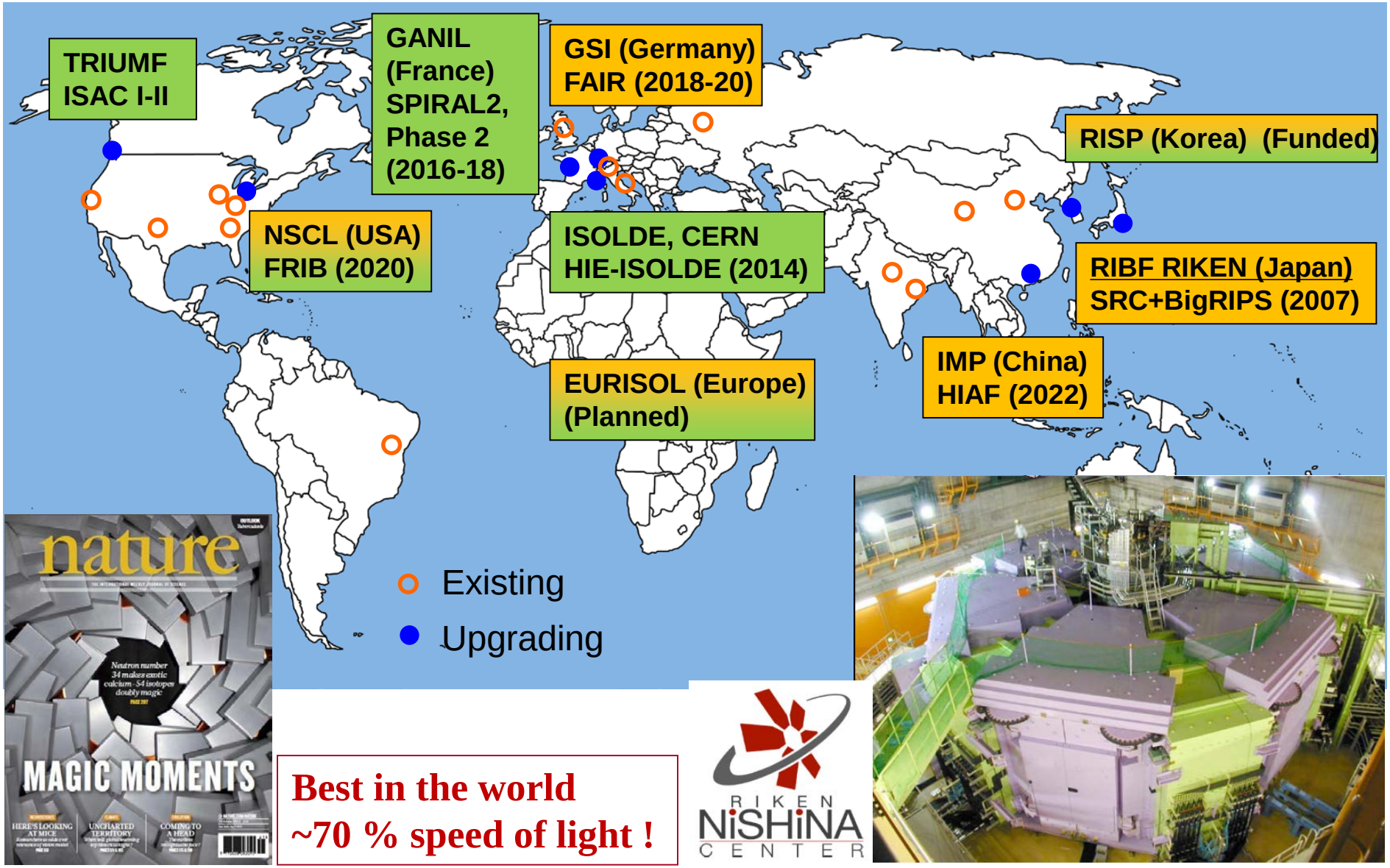


(1985)

~ 1500 nuclei

http://www.nishina.riken.go.jp/index_e.html

Radioactive isotope beam facilities



Best in the world
~70 % speed of light !

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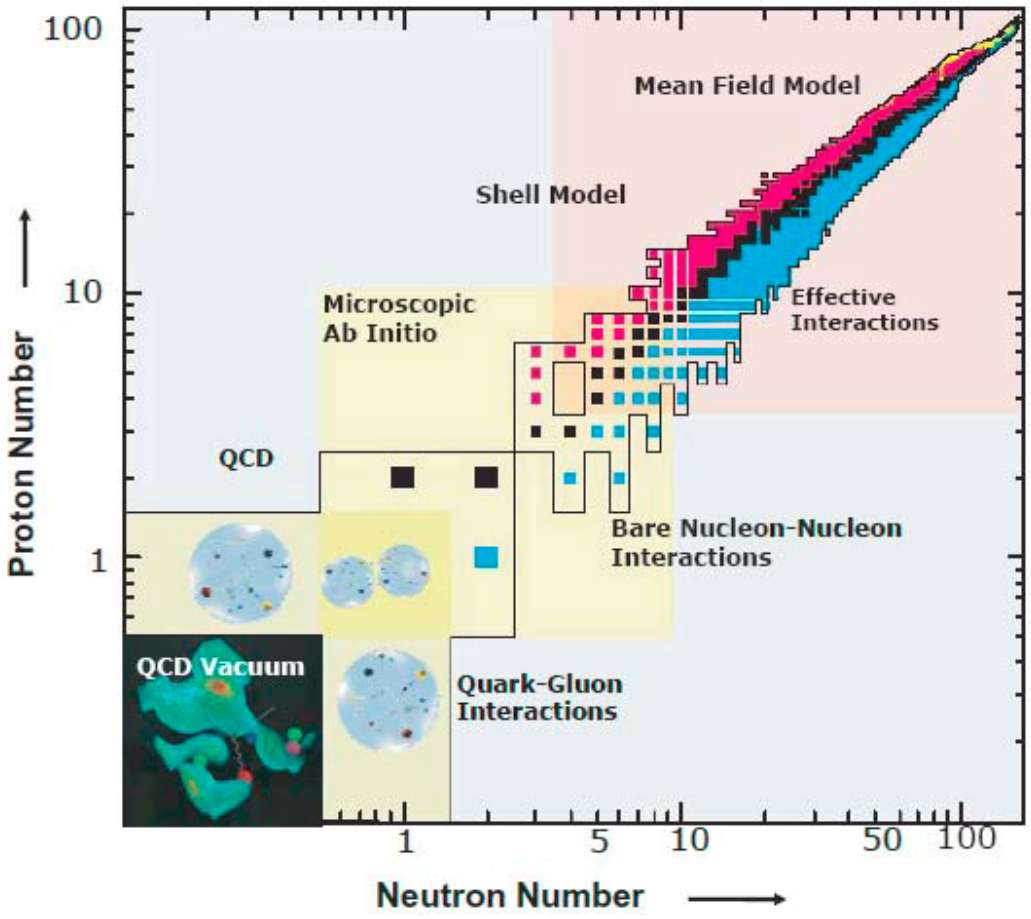
Bottom-up approach to nuclear structure

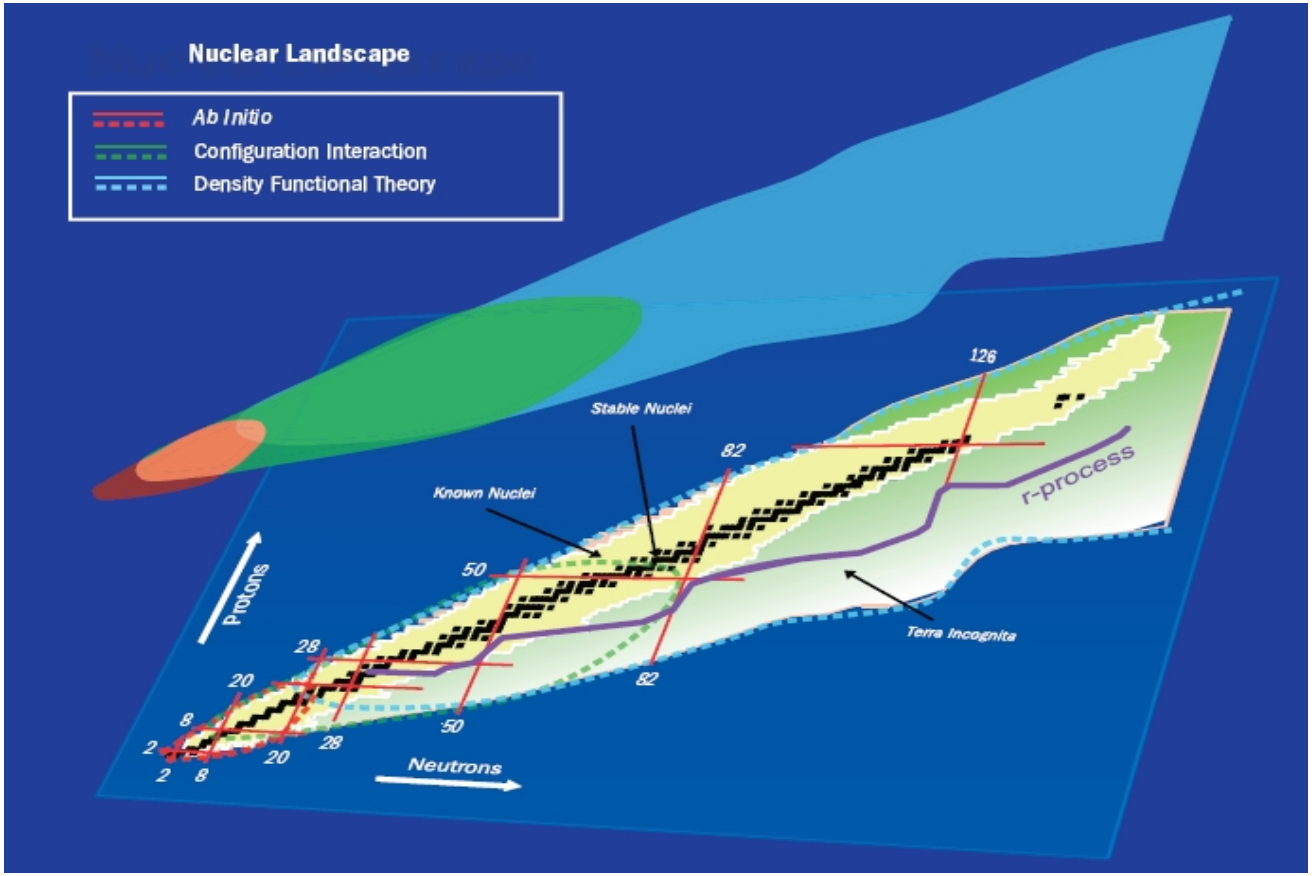


- *"Although QCD is the basic theory of strong interactions, other models must take over for a proper description of the low-energy nuclear behavior."*
- *"The figure indicates some models used and their region of applicability."*
- *"Note that the regions overlap, we are progressing towards a complete understanding of nuclear structure."*

Proper energy scale & degree of freedom for understanding the proper physics

Nuclear Physics European Collaboration Committee
Long Range Plan 2004

State-of-the-art nuclear theories



http://www.unedf.org/

- Density functional theory (DFT) aims at understanding both ground-state and excited-state properties of thousands of nuclei in a consistent and predictive way.

Nuclear many-body problem

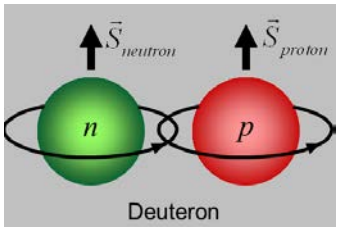
Nuclear *N*-particle system

- Time-dependent Schrödinger/Dirac equation (in this talk $\hbar = c = 1$)

$$i\frac{\partial \Psi(t)}{\partial t} = \hat{H}\Psi(t)$$

- Stationary equation

$$\hat{H}\Psi(x_1, x_2, \ldots, x_N) = E\Psi(x_1, x_2, \ldots, x_N)$$



where $x_i = (\mathbf{r}_i, \sigma_i, \tau_i)$ stands for the **spatial**, **spin**, and **isospin** coordinates.

The problem becomes extremely difficult when $N = 4, 5, 6, \ldots$

- However, the ***N***-particle wave function contains a great deal of information, which is **irrelevant** to most of important physical properties.
- It is very advantageous to introduce the **density matrices**, defined from the many-body wave function by **integrating out** much of **redundant** information.

One-body local density & DFT

One-body local density (a function in 3D space, independent of ***N***)

$$\rho(\mathbf{r}) = \sum_{\sigma,\tau} \int |\Psi(x, x_2, \ldots, x_N)|^2 \mathrm{d}x_2 \ldots \mathrm{d}x_N$$

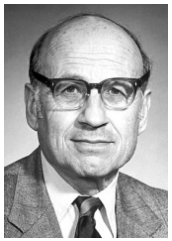
- experimental observable
- with transparent physical meaning
- easily visualized

http://www.nishina.riken.go.jp/index_e.html

The aim of density functional theory (DFT) is

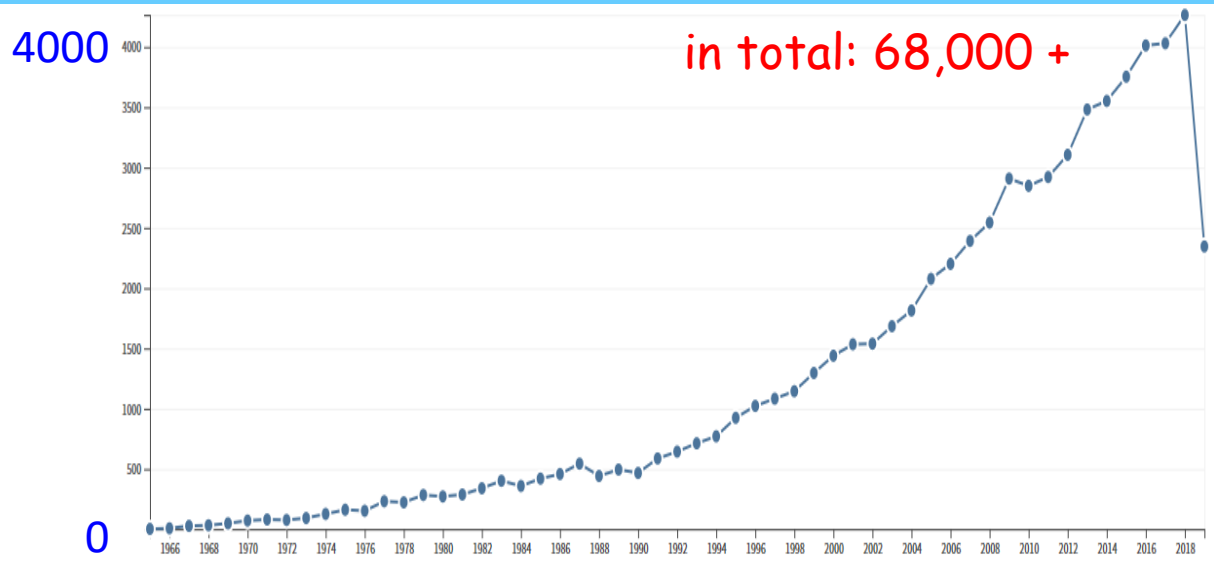
- to reduce the many-body quantum mechanical problem formulated in terms of ***N***-particle wave functions **Ψ** to the one-particle level with the local density distribution **ρ(r)**.

Impacts of DFT



Nobel Prize 1998

"for his development of the density-functional theory"

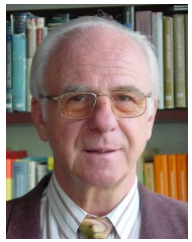


Number of annual citations of HK1964 & KS1965
data from Web of Science

- *"A work of fundamental importance is usually much quoted directly after is publication, but no longer so when it has entered textbooks and has become canonized.* ***Why did this not happen to the Hohenberg-Kohn paper?****"*
- *"Actually the HK theorem is a rather* ***unusual kind of theorem****, that resists an easy interpretation, and that has still* ***a touch of mystery****."*

—— *Werner Kutzelnigg*

J. Mol. Struct. **768**, 163 (2006)



Kohn's Nobel Lecture

Nobel Lecture: Electronic structure of matter—wave functions and density functionals*

W. Kohn

Department of Physics, University of California, Santa Barbara, California 93106

Reviews of Modern Physics, Vol. 71, No. 5, October 1999 0034-6861/99/71(5)/1253(14)/$17.80

CONTENTS

DFT by Legendre transformation

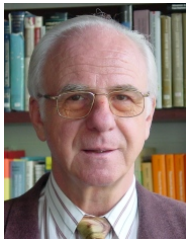
ELSEVIER

Journal of Molecular Structure: THEOCHEM 768 (2006) 163–173

THEO CHEM

www.elsevier.com/locate/theochem

Density functional theory in terms of a Legendre transformation for beginners



Werner Kutzelnigg *

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Available online 22 May 2006

Abstract

The derivation of the Hohenberg–Kohn (HK) theorem by means of a simplified version of Lieb's Legendre transformation is presented, with the stress on physically problematic aspects, and caring about the definition of the domains of the respective functionals only to the extent, that this is absolutely necessary. The take-home lesson consists in a critical analysis of some statements often found in the DFT literature. As a simple illustration for a Legendre transformation we discuss that in parameter space for the family of n-electron isoelectronic atomic ions, with the nuclear charge as parameter.

Hohenberg-Kohn theorem

HK original paper [*Phys. Rev.* **136**, B864 (1964)]

- We develop an **exact formal variational principle** for the ground-state energy E, in which the density $\rho(\mathbf{r})$ is the variable function.
- Into this principle enters **a universal functional** $F_{HK}[\rho(\mathbf{r})]$, which applies to all electronic systems in their ground state no matter what the external potential $u(\mathbf{r})$ is.
- The main objective of theoretical considerations is a description of this functional. **Once known**, it is relatively easy to determine the ground-state energy in a given external potential.

Basic lemma of HK [*Nobel Lecture*]

- The ground-state density $\rho(\mathbf{r})$ of a bound system of interacting electrons in some external potential $u(\mathbf{r})$ determines this potential **uniquely**.

Figure 1. Creators of density functional theory. Walter Kohn (left, in 1962) and his two postdoctoral fellows, Pierre Hohenberg (middle, in 1965) and Lu Sham (right, undated), produced their theory in 1964 and 1965. (Photographs courtesy of Walter Kohn and the John Simon Guggenheim Memorial Foundation, Pierre Hohenberg, and Lu Sham.)

Photos: Zangwill, *Phys. Today* **68**(7), 34 (2015)

Proof of Hohenberg-Kohn theorem (I)

- In proving their theorem, Hohenberg and Kohn considered a collection of **an arbitrary number of electrons** enclosed in a large box, moving under the influence of **an external potential *u*(r)** and the **mutual Coulomb repulsion**.

- Hamiltonian with an external field

$$\hat{H}_u = \hat{T} + \hat{V}_{ee} + \hat{U} \qquad \text{with} \qquad \hat{U} = \int \mathrm{d}x\, \psi^\dagger(x) u(\mathbf{r}) \psi(x)$$

- Schrödinger equation

$$\hat{H}_u \Psi_u(x_1, x_2, \ldots, x_N) = E_u \Psi_u(x_1, x_2, \ldots, x_N)$$

- One-body local density

$$\rho(\mathbf{r}) = \sum_{\sigma,\tau} \int |\Psi(x, x_2, \ldots, x_N)|^2 \mathrm{d}x_2 \ldots \mathrm{d}x_N$$

- ✓ Obviously, Ψ_u and $\rho(\mathbf{r})$ are uniquely determined by $u(\mathbf{r})$.

To prove $u(\mathbf{r})$ is uniquely determined by $\rho(\mathbf{r})$

also see Petkov & Stoitsov, *Nuclear Density Functional Theory* (Clarendon Press, Oxford, 1991)

Proof of Hohenberg-Kohn theorem (II)

- Assume that another potential $u'(\mathbf{r})$ leads to the ground-state wave function $\Psi_{u'}$ and the energy $E_{u'}$, but gives rise to the same density $\rho'(\mathbf{r}) = \rho(\mathbf{r})$.

reductio ad absurdum
归谬法/帰謬法/귀류법

- According to **Rayleigh-Ritz minimal principle**

$$E_{u'} = \langle \Psi_{u'} | \hat{H}_{u'} | \Psi_{u'} \rangle < \langle \Psi_u | \hat{H}_{u'} | \Psi_u \rangle = E_u + \langle \Psi_u | \hat{U}' - \hat{U} | \Psi_u \rangle$$

i.e.,

$$E_{u'} < E_u + \int \mathrm{d}\mathbf{r}[u'(\mathbf{r}) - u(\mathbf{r})]\rho(\mathbf{r})$$

- Exactly, in the same way, one gets

$$E_u < E_{u'} + \int \mathrm{d}\mathbf{r}[u(\mathbf{r}) - u'(\mathbf{r})]\rho(\mathbf{r})$$

$$E_u + E_{u'} < E_u + E_{u'}$$

$$\rho'(\mathbf{r}) \neq \rho(\mathbf{r})$$

- Therefore, $u(\mathbf{r})$ is uniquely determined by $\rho(\mathbf{r})$, so are Hamiltonian H_u, wave function Ψ_u, and the expectation values of all operators of interest.

HK variational principle (I)

- In general, one can obtain the ground-state energy E_u of H_u by

$$E_u = \min_{\tilde{\Psi}} \langle \tilde{\Psi} | \hat{T} + \hat{V}_{ee} + \hat{U} | \tilde{\Psi} \rangle$$

Two-step constrained search method

also cf. Levy, *PRA* **26**, 1200 (1982); Lieb, *Int. J. Quantum Chem.* **24**, 243 (1983)

1. Fix a trial ground-state density $\tilde{\rho}(\mathbf{r})$, denoting $\tilde{\Psi}_{\tilde{\rho}}$ the class of trial wave functions with this density

$$E_u[\tilde{\rho}(\mathbf{r})] = \min_{\tilde{\Psi}_{\tilde{\rho}}} \langle \tilde{\Psi}_{\tilde{\rho}} | \hat{T} + \hat{V}_{ee} + \hat{U} | \tilde{\Psi}_{\tilde{\rho}} \rangle = F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r}) \tilde{\rho}(\mathbf{r}) \mathrm{d}\mathbf{r}$$

   where

$$F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] = \min_{\tilde{\Psi}_{\tilde{\rho}}} \langle \tilde{\Psi}_{\tilde{\rho}} | \hat{T} + \hat{V}_{ee} | \tilde{\Psi}_{\tilde{\rho}} \rangle$$

2. Minimize E_u over all $\tilde{\rho}(\mathbf{r})$

$$E_u = \min_{\tilde{\rho}} \left\{ F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r}) \tilde{\rho}(\mathbf{r}) \mathrm{d}\mathbf{r} \right\}$$

- $F_{\mathrm{HK}}[\rho(\mathbf{r})]$ requires no explicit knowledge of $u(\mathbf{r})$.
- It is **a universal functional** of the density $\rho(\mathbf{r})$.

HK variational principle (II)

- **HK variation principle**

$$\delta E_u = \int \mathrm{d}\mathbf{r} \left\{ \frac{\delta F_{\mathrm{HK}}}{\delta \tilde{\rho}(\mathbf{r})} + u(\mathbf{r}) - \mu \right\} \delta \tilde{\rho}(\mathbf{r}) = 0$$

- **Euler-Lagrange equations**

$$\left\{ \frac{\delta F_{\mathrm{HK}}}{\delta \tilde{\rho}(\mathbf{r})} + u(\mathbf{r}) - \mu \right\} \delta \tilde{\rho}(\mathbf{r}) = 0$$

with Lagrange multiplier $\boldsymbol{\mu}$, **chemical potential**.

Non-interaction system (I)

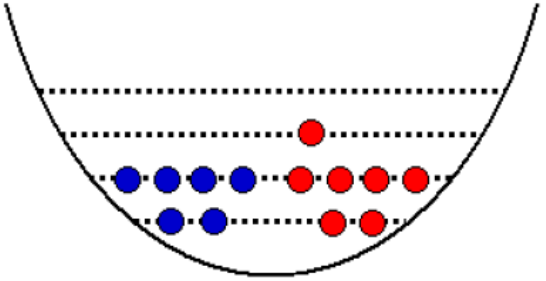
***Exercise*: Non-interacting system**

$$F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] \Rightarrow T_0[\tilde{\rho}(\mathbf{r})] = \min_{\tilde{\Psi}_{\tilde{\rho}}} \langle \tilde{\Psi}_{\tilde{\rho}} | \hat{T} | \tilde{\Psi}_{\tilde{\rho}} \rangle$$

$$\left\{ \frac{\delta T_0}{\delta \tilde{\rho}(\mathbf{r})} + u(\mathbf{r}) - \mu \right\} \delta\tilde{\rho}(\mathbf{r}) = 0$$

- However, even in this simple case, the functional $T_0[\rho(\mathbf{r})]$ is **unknown**.

We are in the fortunate situation that



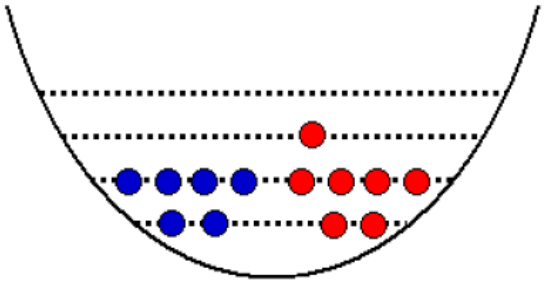
- One-body local density $\rho(\mathbf{r}) = \sum_{i=1}^{N} \varphi_i^*(\mathbf{r}) \varphi_i(\mathbf{r})$
- Expectation value of kinetic energy $T_0 = \langle \hat{T} \rangle = \sum_{i=1}^{N} \langle \varphi_i | -\frac{1}{2M} \nabla^2 | \varphi_i \rangle$
- Thus $\frac{\delta T_0}{\delta \varphi_i^*(\mathbf{r})} = -\frac{1}{2M} \nabla^2 \varphi_i(\mathbf{r})$

$$\frac{\delta T_0}{\delta \varphi_i^*(\mathbf{r})} = \int \mathrm{d}\mathbf{r}' \frac{\delta T_0}{\delta \rho(\mathbf{r}')} \frac{\delta \rho(\mathbf{r}')}{\delta \varphi_i^*(\mathbf{r})} = \frac{\delta T_0}{\delta \rho(\mathbf{r})} \varphi_i(\mathbf{r})$$

Non-interaction system (II)

- If we get the solutions of Schrödinger equation exactly

$$\left\{-\frac{1}{2M}\nabla^2 + u(\mathbf{r}) - \epsilon_i\right\}\varphi_i(\mathbf{r}) = 0$$



we get the solution of the HK variation principle.

$$\left\{\frac{\delta T_0}{\delta\tilde{\rho}(\mathbf{r})} + u(\mathbf{r}) - \mu\right\}\delta\tilde{\rho}(\mathbf{r}) = 0$$

- *"We are so in the curious situation, that we are able to solve the HK variational equations, without even knowing anything about the functional* $\boldsymbol{F_{HK}}$*, nor its derivative (except that they exist)."*

"DFT without a density functional"

Kutzelnigg, *J. Mol. Struct.* **768**, 163 (2006)

Kohn-Sham scheme

- The unknown functional $F_{HK}[\rho(\mathbf{r})]$ is decomposed into two parts
  Phys. Rev. **140**, A1133 (1965)

$$F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] = T_0[\tilde{\rho}(\mathbf{r})] + I[\tilde{\rho}(\mathbf{r})]$$

- **$I[\rho(\mathbf{r})]$ = interaction energy + (T - T_0)** ← Caution: T the actual kinetic energy

- To solve Euler-Lagrange equations for HK variation principle

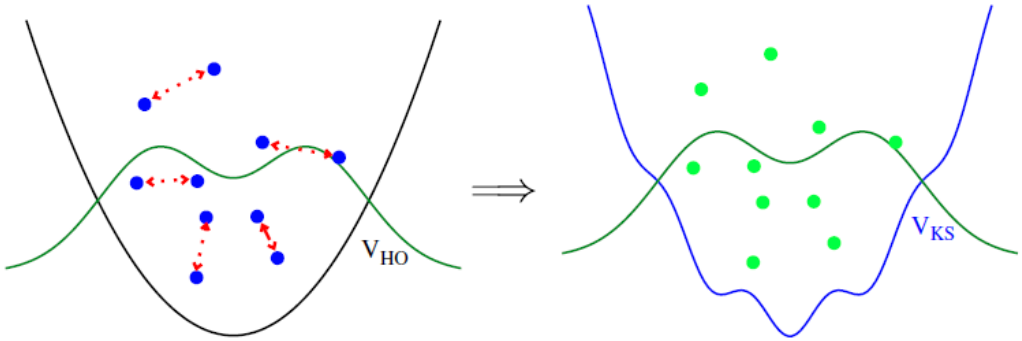
$$\left\{ \frac{\delta T_0}{\delta \tilde{\rho}(\mathbf{r})} + u_{\mathrm{KS}}(\mathbf{r}) - \mu \right\} \delta\tilde{\rho}(\mathbf{r}) = 0 \quad \text{where} \quad u_{\mathrm{KS}}(\mathbf{r}) = u(\mathbf{r}) + \frac{\delta I}{\delta \tilde{\rho}(\mathbf{r})}$$

  by solving **KS equations** (self-consistently)

$$\left\{ -\frac{1}{2M}\nabla^2 + u_{\mathrm{KS}}(\mathbf{r}) - \epsilon_i \right\} \varphi_i(\mathbf{r}) = 0$$

$$I[\tilde{\rho}(\mathbf{r})] = \frac{1}{2}\iint \frac{\tilde{\rho}(\mathbf{r}_1)\tilde{\rho}(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 + E_{\mathrm{xc}}[\tilde{\rho}(\mathbf{r})]$$

always local?



Questions & Discussions (I)

- **All information about the ground state of a Hamiltonian is in the density $\rho(\mathbf{r})$.**

- **$\rho(\mathbf{r}) \rightarrow u(\mathbf{r}) \rightarrow H_u \rightarrow \Psi \rightarrow$ everything (?)**
  - The first **objection** against this argument is that the problem, that **$\rho(\mathbf{r})$** is given, but **$u(\mathbf{r})$** unknown, never arises in practice.
  - Second, whether it is appropriate to call the exact **Ψ** a functional of **ρ** has **no significant conclusions**. Lieb, *Int. J. Quantum Chem.* **24**, 243 (1983)

- Nevertheless, whether **Ψ** a functional of **ρ** is irrelevant for the central issue of DFT, namely the existence of **$F_{HK}[\rho(\mathbf{r})]$**. It has no consequences, and therefore

"it is an empty statement"

Functionals

- **$E[u(\mathbf{r})], F_{HK}[\rho(\mathbf{r})]$** ✓ *vs* **$\Psi[u(\mathbf{r})], \Psi[\rho(\mathbf{r})]$** ✘
- *Functionals have **well-defined domains** and **analytic properties**, that, e.g., allow the construction of Legendre transformations.*

Questions & Discussions (II)

- **Wave-function theory and DFT are two equivalent alternative approaches to solve the *n*-electron problem.**

- There are some similarities:

$$E_u = \min_{\tilde{\Psi}} \langle \tilde{\Psi} | \hat{T} + \hat{V}_{ee} + \hat{U} | \tilde{\Psi} \rangle \qquad E_u = \min_{\tilde{\rho}} \left\{ F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r}) \tilde{\rho}(\mathbf{r}) \mathrm{d}\mathbf{r} \right\}$$

  In both cases one specifies a ***u*(r)** and searches for an infimum, either over a set of wave functions or of densities.

- There are also differences:

  DFT would only lead to ***E*** and ***ρ*(r)**, i.e. to **less information** than that contained in ***E*** and **Ψ**.

"if one is interested in Ψ, even HK have no better suggestion than to solve the Schrödinger equation"

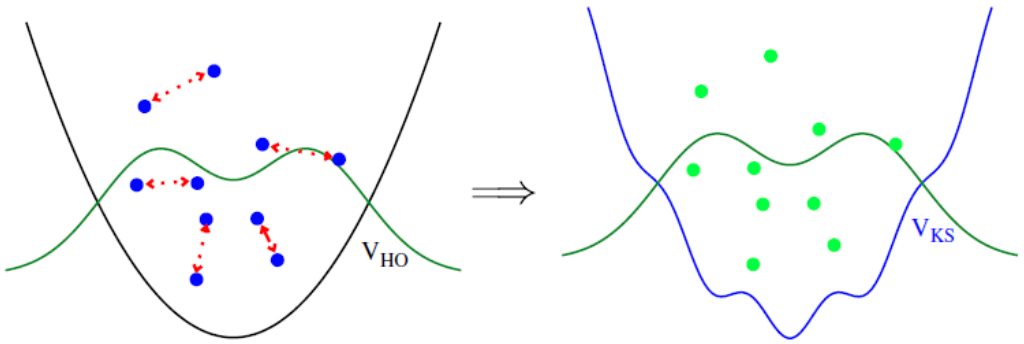
Questions & Discussions (III)

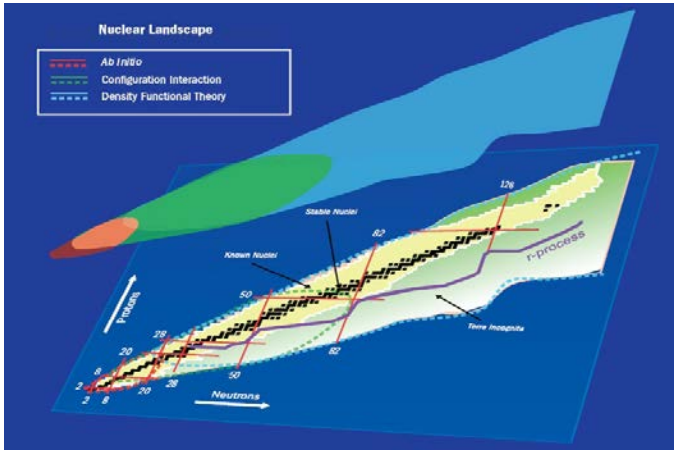
- **(Kohn-Sham) DFT is a mean-field model.**

"no"

- **DFT cannot apply to very light nuclei.**

"it is not true"





Hartree-Fock *vs* DFT

- **Ritz variational principle** and Hartree-Fock theory

$$E_u = \min_{\tilde{\Psi}} \langle \tilde{\Psi} | \hat{T} + \hat{V}_{ee} + \hat{U} | \tilde{\Psi} \rangle$$

HF ➔ BCS ➔ HFB ➔ Quantum Monte-Carlo ➔ …

To search the ground state by using larger and larger sets of trail w.f.

- **HK variational principle** and DFT

$$E_u = \min_{\tilde{\rho}} \left\{ F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r}) \tilde{\rho}(\mathbf{r}) \mathrm{d}\mathbf{r} \right\}$$

$$F_{\mathrm{HK}}[\rho] = T_0[\rho] + E_{\mathrm{H}}[\rho] + E_{\mathrm{x}}^{\mathrm{LDA}}[\rho] + E_{\mathrm{c}}^{\mathrm{LDA}}[\rho] + E_{\mathrm{xc}}^{\mathrm{GGA}}[\rho, |\nabla\rho|] + E_{\mathrm{xc}}^{\mathrm{Meta-GGA}}[\rho, |\nabla\rho|, \nabla^2\rho, \tau] + \cdots$$

To search better and better approximations to EDF

Once F_{HK} is known …

Hohenberg & Kohn, *Phys. Rev.* **136**, B864 (1964)

- Once the universal functional $F_{HK}[\rho(\mathbf{r})]$ is known, it is relatively easy to determine the ground-state energy in a given external potential.

$$E_u = \min_{\tilde{\rho}} \left\{ F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r})\tilde{\rho}(\mathbf{r})\mathrm{d}\mathbf{r} \right\}$$

- Note that

$F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] = \min_{\tilde{\Psi}_{\tilde{\rho}}} \langle \tilde{\Psi}_{\tilde{\rho}} | \hat{T} + \hat{V}_{ee} | \tilde{\Psi}_{\tilde{\rho}} \rangle$ as complicated as $E_u = \min_{\tilde{\Psi}} \langle \tilde{\Psi} | \hat{T} + \hat{V}_{ee} + \hat{U} | \tilde{\Psi} \rangle$

- Alternatively,

$$F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] = \sup_{\tilde{\tilde{u}}} \left\{ E[\tilde{\tilde{u}}(\mathbf{r})] - \int \tilde{\tilde{u}}(\mathbf{r})\tilde{\rho}(\mathbf{r})\mathrm{d}\mathbf{r} \right\}$$

assuming all **$E[u(\mathbf{r})]$** are known

This is not a very realistic assumption.

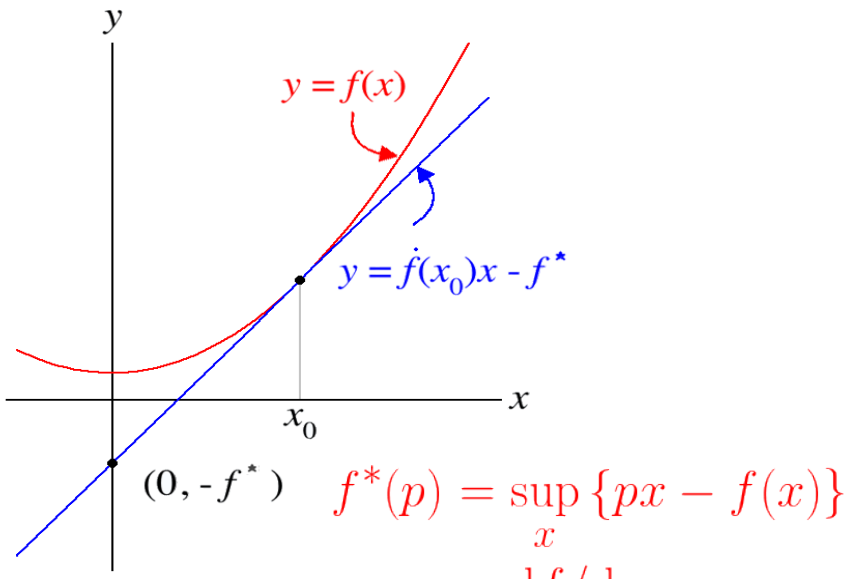
- *Why should we assume that the more difficult problem to know **E(u)** for a family of **u** is solved, if we are interested in the much simpler problem to obtain **E(u)** for a single **u**?*

Kutzelnigg, *J. Mol. Struct.* **768**, 163 (2006)

Mathematical foundations of DFT

The Fundamentals of Density Functional Theory (revised and extended version)

H. Eschrig



$$f^*(p) = \sup_x \{px - f(x)\}$$

$$p = \mathrm{d}f/\mathrm{d}x$$

From wikipedia

Keys

Convex-functional analysis

Legendre transformation

Mathematical foundations of DFT

Functionals

- $E[u(\mathbf{r})]$, $F_{\mathrm{HK}}[\rho(\mathbf{r})]$ ✓ *vs* $\Psi[u(\mathbf{r})]$, $\Psi[\rho(\mathbf{r})]$ ✗
  - *Functionals have **well-defined domains** and **analytic properties**, that, e.g., allow the construction of Legendre transformations.*

$$L^k(\mathbb{R}^3) := \left\{ \int |f(\mathbf{r})|^k \mathrm{d}\mathbf{r} \right\}^{1/k} < \infty$$

From $E[u(\mathbf{r})]$ to $F_{\mathrm{HK}}[\rho(\mathbf{r})]$

- $E[u(\mathbf{r})]$ is a **concave functional** in $u \in L^{3/2} + L^{\infty}$
- Legendre transformation is well defined

$$F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] = \sup_{\tilde{\tilde{u}}} \left\{ E[\tilde{\tilde{u}}(\mathbf{r})] - \int \tilde{\tilde{u}}(\mathbf{r})\tilde{\rho}(\mathbf{r})\mathrm{d}\mathbf{r} \right\}$$

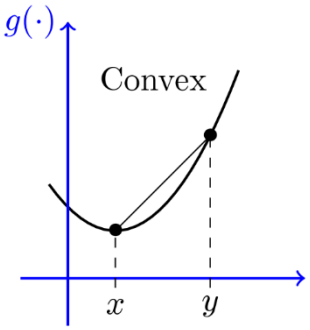
- Restriction to **Coulomb** potentials is essential.
- HK theorem would **not** hold **for arbitrary** potentials.

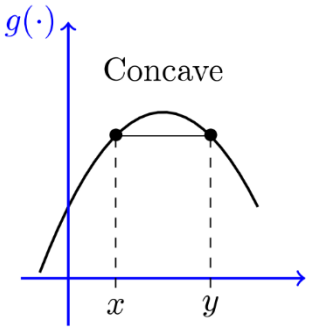
Lieb (1983)

From $F_{\mathrm{HK}}[\rho(\mathbf{r})]$ to $E[u(\mathbf{r})]$

- $F_{\mathrm{HK}}[\rho(\mathbf{r})]$ is a **convex functional** in $\rho \in L^3 \cap L^1$
- Legendre transformation is well defined

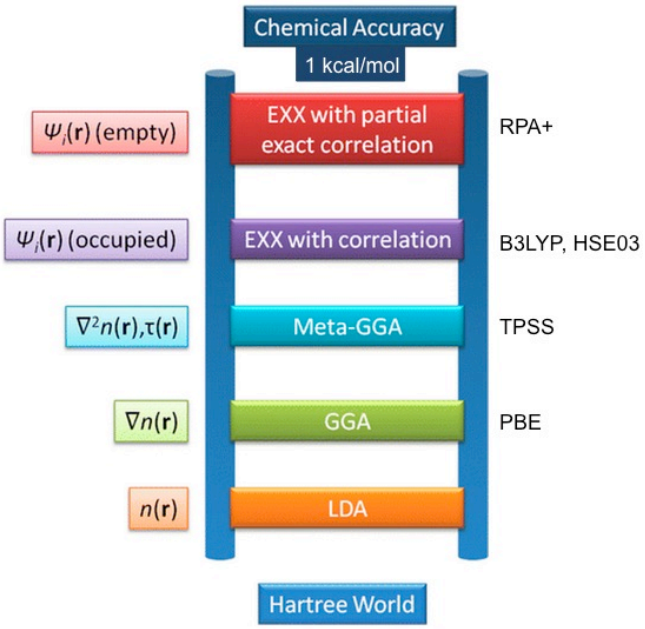
$$E[u(\mathbf{r})] = \inf_{\tilde{\rho}} \left\{ F_{\mathrm{HK}}[\tilde{\rho}(\mathbf{r})] + \int u(\mathbf{r})\tilde{\rho}(\mathbf{r})\mathrm{d}\mathbf{r} \right\}$$





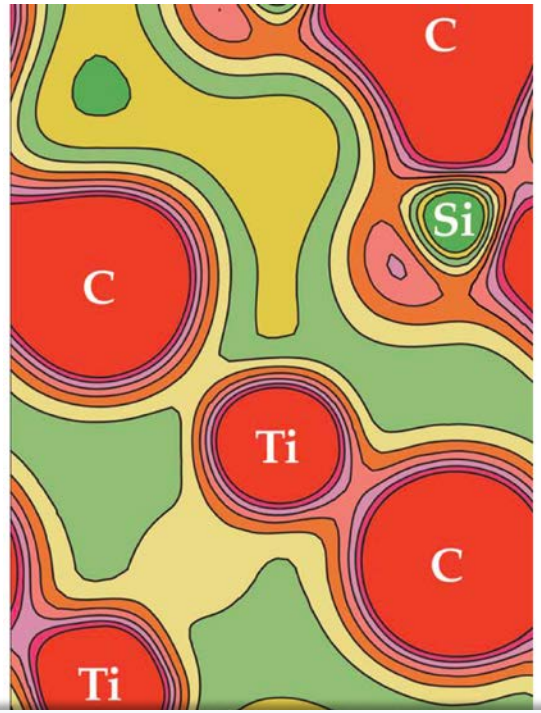
Lieb, *Int. J. Quantum Chem.* **24**, 243 (1983); Eschrig (2003)

The legacy of DFT



Jacob's Ladder Perdew & Schmidt (2001)
http://www.sas.upenn.edu/~jianmint/Research/

Zangwill, *Phys. Today* **68**(7), 34 (2015)



A half century of **density functional theory**

Andrew Zangwill

Today's most popular method for calculating the electronic structure of atoms, molecules, liquids, solids, and plasmas began as a bold hypothesis: The electron density distribution completely characterizes the ground state of a many-electron system.

The legacy of DFT

- *"One could argue that the algorithms implemented in DFT programs reflect a long sequence of approximations and extensions made by many individuals to the original Hartree-Fock method."*
- *"DFT provides both **the scientific justification** and **the basis for understanding the meaning behind these algorithms**."*

DFT to isolated nucleus

Nucleus is a self-bound system (without external potential)

- It is somewhat useless to use the ground-state density in the laboratory frame, because $\rho(\mathbf{r}) = N/V \rightarrow 0$ $(V \rightarrow \infty)$.
- DFT theorem for the **intrinsic density** $\rho_{\text{intr.}}(\mathbf{r})$ (a *wave-packet* state)

$$|\Psi\rangle = |\Phi\rangle \otimes |\chi\rangle$$

where Φ indicates the **intrinsic state** and χ defines the **spurious motion**.

See, e.g.,
Review

REVIEWS OF MODERN PHYSICS, VOLUME 88, OCTOBER–DECEMBER 2016

Time-dependent density-functional description of nuclear dynamics

Nakatsukasa, Matsuyanagi, Matsuo, Yabana, *RMP* **88**, 045004 (2016)

Open questions:

- What is the domain of $\rho_{\text{intr.}}(\mathbf{r})$?
- Is $F[\rho_{\text{intr.}}(\mathbf{r})]$ strictly convex in this domain?

Contents

Fundamentals of Density Functional Theory

- Interesting viewpoints on **DFT**
- Hohenberg-Kohn (**HK**) theorem
- Kohn-Sham (**KS**) scheme
- *Discussion*: some open issues

Nuclear DFT and applications

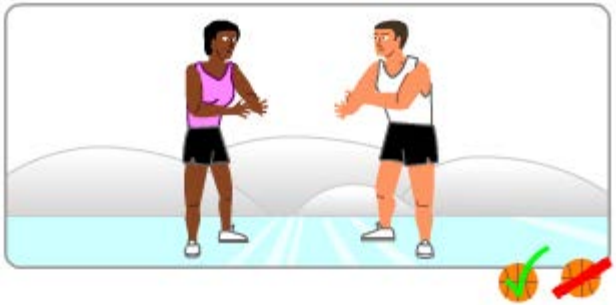
- Covariant Density Functional Theory (**CDFT**)
- *Application*: Nuclear tensor force and its effects

Connections to Quantum Field Theory

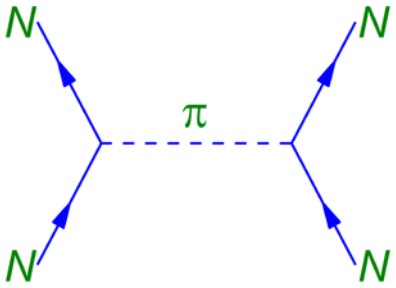
- Energy density functional and effective action in **QFT**
- Functional Renormalization Group (**FRG**)
- *Application*: φ^4-theory in zero dimension

Nucleon-nucleon interaction

Nucleon-nucleon interaction



http://www.particleadventure.org/



Nobel Prize 1949

Bonn meson-exchange model for NN interaction

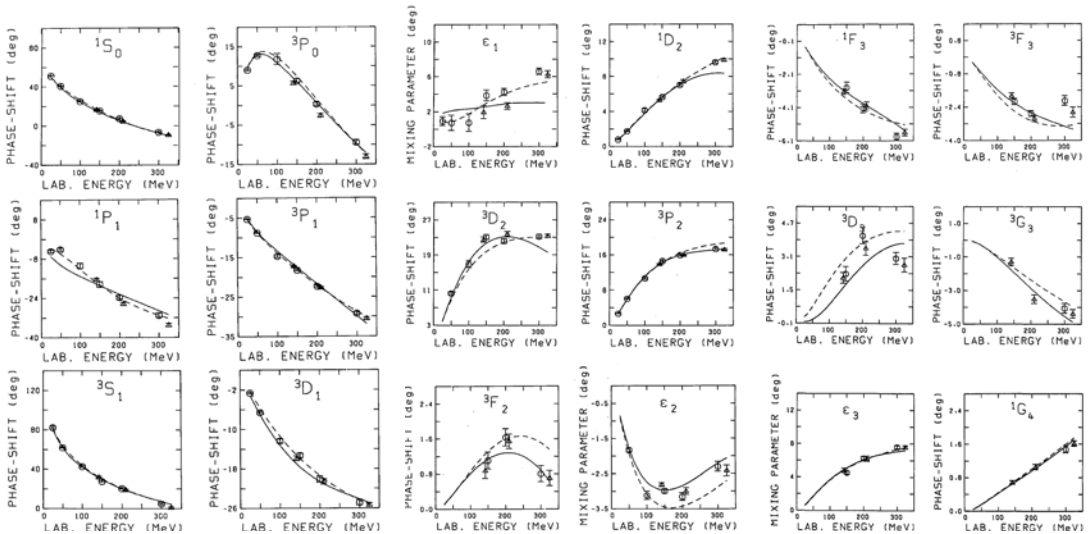


Table 5

Meson parameters used in the relativistic (energy-independent) momentum space one-boson-exchange potential (OBEPQ)

	$g_\alpha^2/4\pi$; $[f_\alpha/g_\alpha]$	$g_\alpha^2/4\pi(k^2=0)$	m_α [MeV]	Λ_α [GeV]	n_α
π	14.6	14.27	138.03	1.3	1
ρ	0.81; [6.1]	0.43	769	2.0	2
η	5	3.75	548.8	1.5	1
ω	20; [0.0]	10.6	782.6	1.5	1
δ	1.1075	0.64	983	2.0	1
σ	8.2797 [a]	7.07	550 [a]	2.0	1

Machleidt, Holinde, Elster, *Phys. Rep.* **149**, 1 (1987)

Covariant density functional theory (I)

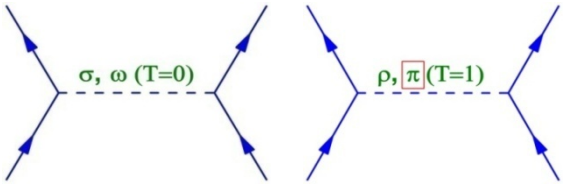
Effective Lagrangian density: starting point of CDFT

$$\mathscr{L} = \bar{\psi}\left[i\gamma^\mu\partial_\mu - M - g_\sigma\sigma - \gamma^\mu\left(g_\omega\omega_\mu + g_\rho\vec{\tau}\cdot\vec{\rho}_\mu + e\frac{1-\tau_3}{2}A_\mu\right) - \frac{f_\pi}{m_\pi}\gamma_5\gamma^\mu\partial_\mu\vec{\pi}\cdot\vec{\tau}\right]\psi$$
$$+\frac{1}{2}\partial^\mu\sigma\partial_\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu - \frac{1}{4}\vec{R}_{\mu\nu}\cdot\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^\mu\cdot\vec{\rho}_\mu$$
$$+\frac{1}{2}\partial_\mu\vec{\pi}\cdot\partial^\mu\vec{\pi} - \frac{1}{2}m_\pi^2\vec{\pi}\cdot\vec{\pi} - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}$$

where $\Omega^{\mu\nu} \equiv \partial^\mu\omega^\nu - \partial^\nu\omega^\mu$, $\vec{R}^{\mu\nu} \equiv \partial^\mu\vec{\rho}^\nu - \partial^\nu\vec{\rho}^\mu$, $F^{\mu\nu} \equiv \partial^\mu A^\nu - \partial^\nu A^\mu$

- Legendre transformation

$$\mathcal{H} = T^{00} = \frac{\partial\mathcal{L}}{\partial\dot{\phi}_i}\dot{\phi}_i - \mathcal{L}$$



where ϕ_i represent the nucleon, meson, and photon fields.

- The **Lorentz covariance** is taken into account.

See, e.g.,
Serot & Walecka, *The Relativistic Nuclear Many Body Problem* (1986)
Bouyssy *et al.*, *Phys. Rev. C* **36**, 380 (1987); Long, Giai, Meng, *Phys. Lett. B* **640**, 150 (2006)

Covariant density functional theory (II)

- The **Hamiltonian density** then is obtained as

$$\mathcal{H} = \mathcal{H}_N + \mathcal{H}_\sigma + \mathcal{H}_\omega + \mathcal{H}_\rho + \mathcal{H}_\pi + \mathcal{H}_A + \mathcal{H}_{\text{int.}}$$

where the contributions from nucleon, meson and photon fields are

$$\begin{aligned}
\mathcal{H}_N &= \bar{\psi}\left[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M\right]\psi, \\
\mathcal{H}_{\text{int.}} &= \bar{\psi}\left[g_\sigma\sigma + g_\omega\gamma^\mu\omega^\mu + g_\rho\gamma^\mu\vec{\tau}\cdot\vec{\rho}^\mu + \frac{f_\pi}{m_\pi}\gamma_5\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}\vec{\pi}\cdot\vec{\tau} + e\frac{1-\tau_3}{2}\gamma^\mu A^\mu\right]\psi, \\
\mathcal{H}_\sigma &= +\frac{1}{2}\dot{\sigma}^2 + \frac{1}{2}\boldsymbol{\nabla}\sigma\cdot\boldsymbol{\nabla}\sigma + \frac{1}{2}m_\sigma^2\sigma^2, \\
\mathcal{H}_\omega &= -\frac{1}{2}\Omega^{0\nu}\dot{\omega}_\nu + \frac{1}{2}\Omega^{i\nu}\partial_i\omega_\nu - \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu, \\
\mathcal{H}_\rho &= -\frac{1}{2}\vec{R}^{0\nu}\cdot\dot{\vec{\rho}}_\nu + \frac{1}{2}\vec{R}^{i\nu}\cdot\partial_i\vec{\rho}_\nu - \frac{1}{2}m_\rho^2\vec{\rho}_\mu\cdot\vec{\rho}^\mu \\
\mathcal{H}_\pi &= +\frac{1}{2}\dot{\vec{\pi}}^2 + \frac{1}{2}\boldsymbol{\nabla}\vec{\pi}\cdot\boldsymbol{\nabla}\vec{\pi} + \frac{1}{2}m_\pi^2\vec{\pi}^2, \\
\mathcal{H}_A &= -\frac{1}{2}F^{0\nu}\dot{A}_\nu + \frac{1}{2}F^{i\nu}\partial_i A_\nu.
\end{aligned}$$

Covariant density functional theory (III)

- Trial wave function (Slater determinant: **mean-field approximation**)

$$|\Phi_0\rangle = \prod_k c_k^\dagger |0\rangle$$

Energy functional of the system

$$E[\rho] = \langle\Phi_0|\mathcal{H}|\Phi_0\rangle = E_k + E_\sigma^D + E_\omega^D + E_\rho^D + E_A^D + E_\sigma^E + E_\omega^E + E_\rho^E + E_\pi^E + E_A^E$$

"***D***" represents the **direct terms** and "***E***" represents the **exchange terms**.

"There is no direct term of ***π****. Why?"*

Hartree approximation (I)

Relativistic Mean Field (RMF) = relativistic Hartree approximation

- Energy functional of the system

See, e.g.,
Meng et al., Prog. Part. Nucl. Phys. **57**, 470 (2006)

$$
\begin{aligned}
E_{\mathrm{RMF}}[\rho] &= \langle\Phi_0|\mathcal{H}|\Phi_0\rangle \\
&= \mathrm{Tr}[\beta(-i\gamma\cdot\nabla + M)\rho] \\
&\quad + \mathrm{Tr}\left[\beta\left(g_\sigma\sigma + g_\omega\gamma^\mu\omega^\mu + g_\rho\gamma^\mu\vec{\tau}\cdot\vec{\rho}^\mu + e\frac{1-\tau_3}{2}\gamma^\mu A^\mu\right)\rho\right] \\
&\quad + \int d\mathbf{r}\left\{\frac{1}{2}\dot{\sigma}^2 + \frac{1}{2}\nabla\sigma\cdot\nabla\sigma + \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{2}\Omega^{0\nu}\dot{\omega}_\nu + \frac{1}{2}\Omega^{i\nu}\partial_i\omega_\nu - \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu\right. \\
&\quad \left. - \frac{1}{2}\vec{R}^{0\nu}\cdot\dot{\vec{\rho}}_\nu + \frac{1}{2}\vec{R}^{i\nu}\cdot\partial_i\vec{\rho}_\nu - \frac{1}{2}m_\rho^2\vec{\rho}_\mu\cdot\vec{\rho}^\mu - \frac{1}{2}F^{0\nu}\dot{A}_\nu + \frac{1}{2}F^{i\nu}\partial_i A_\nu\right\}
\end{aligned}
$$

- time reversal symmetry ➔ only time-like components of $\omega_\mu,\ \vec{\rho}_\mu,\ A_\mu$
- no isospin-mix ➔ only third component of $\vec{\tau},\ \vec{\rho}_\mu$
- stationary states ➔ only space derivatives of meson fields

Hartree approximation (II)

- The variation principle with respect to $\phi_i^\dagger$ leads to the **Dirac equation**

$$[\alpha \cdot \mathbf{p} + V(\mathbf{r}) + \beta\,(M + S(\mathbf{r}))]\,\phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r})$$

with $S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r})$ and $V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \tau_3 \rho(\mathbf{r}) + e\dfrac{1-\tau_3}{2} A(\mathbf{r})$

- The variation principle with respect to $\sigma,\ \omega_0,\ \rho_0^3,\ A_0$ leads to the **Klein-Gordon equations**

$$(-\Delta + m_\sigma^2)\sigma(\mathbf{r}) = -g_\sigma \rho_s(\mathbf{r}) \qquad (-\Delta + m_\omega^2)\omega(\mathbf{r}) = g_\omega \rho_v(\mathbf{r})$$

$$(-\Delta + m_\rho^2)\rho(\mathbf{r}) = g_\rho \rho_3(\mathbf{r}) \qquad -\Delta A_0(\mathbf{r}) = e\rho_c(\mathbf{r})$$

with the **local densities**

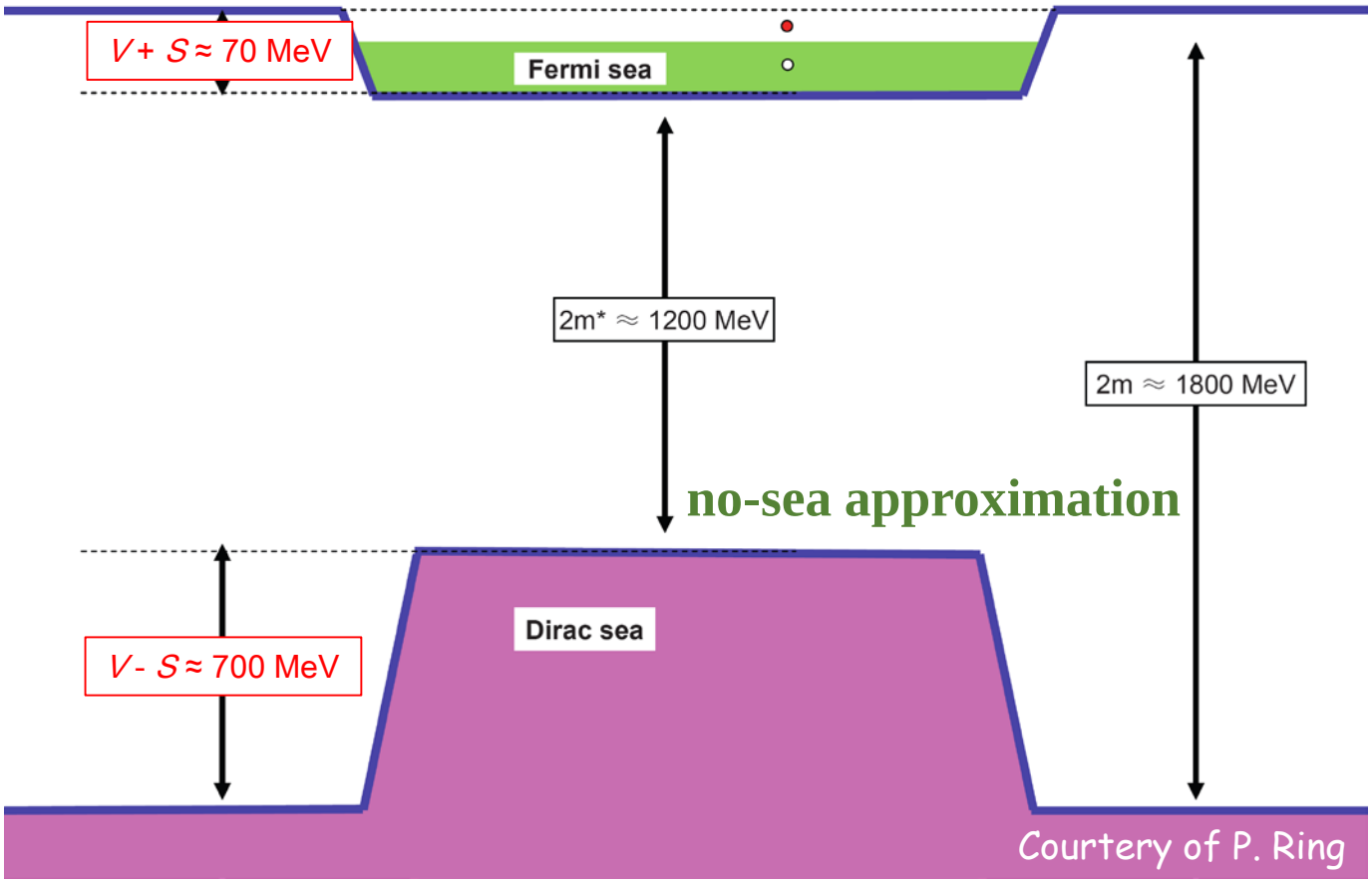
$$\rho_s(\mathbf{r}) = \sum_{i=1}^{A} \bar{\psi}_i(\mathbf{r})\psi_i(\mathbf{r}) \qquad \rho_v(\mathbf{r}) = \sum_{i=1}^{A} \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})$$

$$\rho_3(\mathbf{r}) = \sum_{i=1}^{A} \psi_i^\dagger(\mathbf{r})\tau_3\psi_i(\mathbf{r}) \qquad \rho_c(\mathbf{r}) = \sum_{p=1}^{Z} \psi_p^\dagger(\mathbf{r})\psi_p(\mathbf{r})$$

- To solve the equations in a **self-consistent** (**iterative**) way.

Nuclear potentials in relativistic models

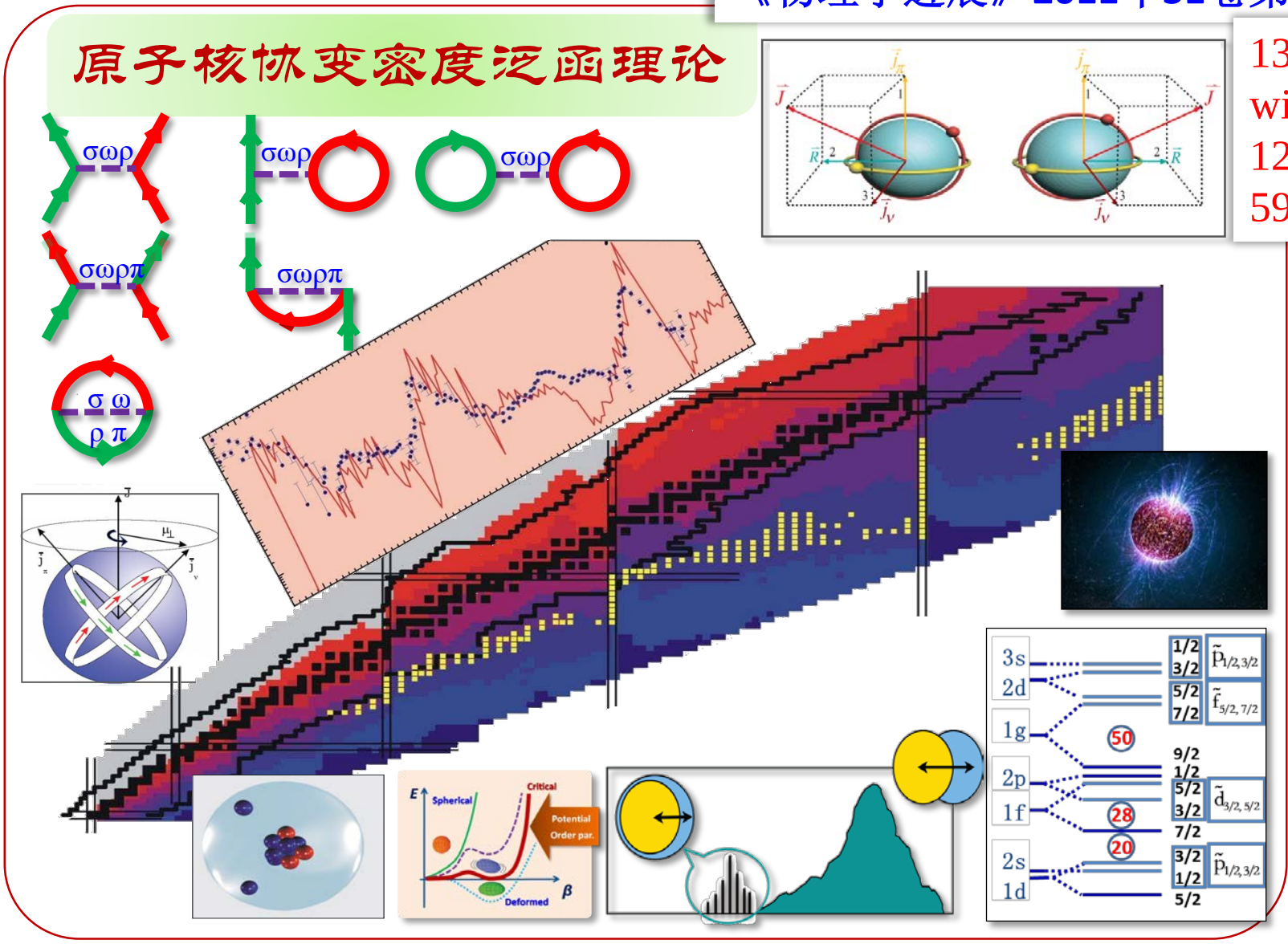
- The scalar and vector potentials are both very big in amplitude, but with opposite signs: ***S*(r) < 0** and ***V*(r) > 0**.
- This results in a shallow **Fermi sea** and a deep **Dirac sea**, the latter is responsible for the **large spin-orbit coupling**.



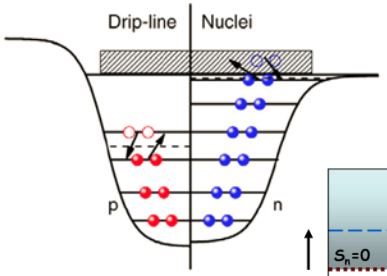
Another nuclear chart

《物理学进展》2011年31卷第4期

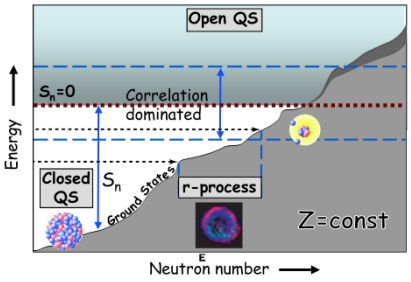
138 pp
with
122 figs
595 refs



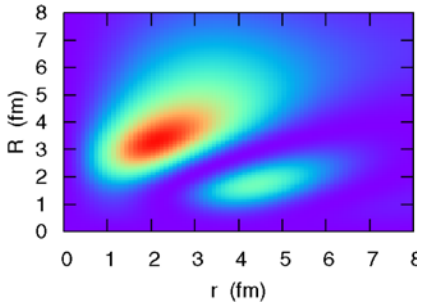
Physics of exotic nuclei

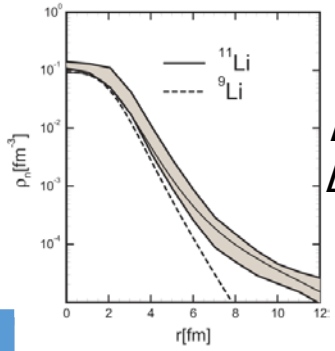


Weakly-bound



Threshold
Continuum
Open Q.S.

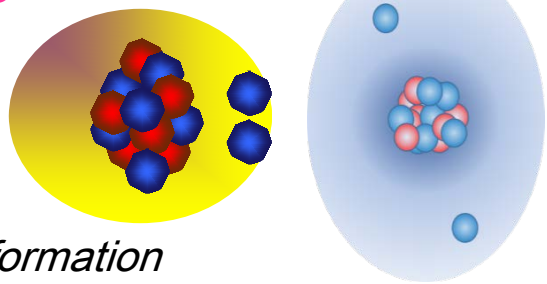




Halo

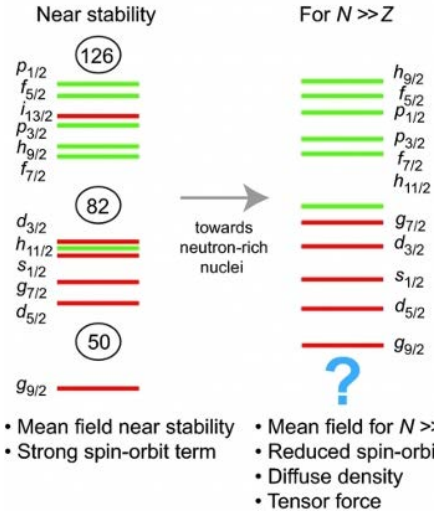
Large spatial ext.
Low-density N.M.
2N correlation

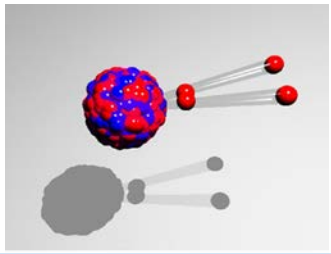
Halo



Deformation
Shape decoupling

Shell evolution

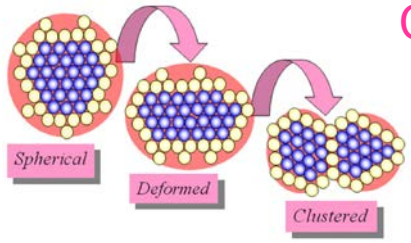


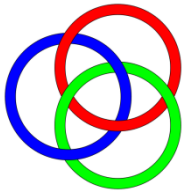


New radioact.

1p emission
2p emission
2n emission

Clustering



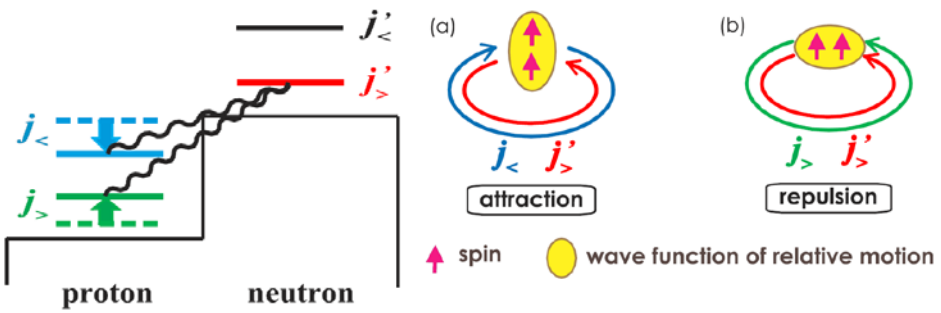


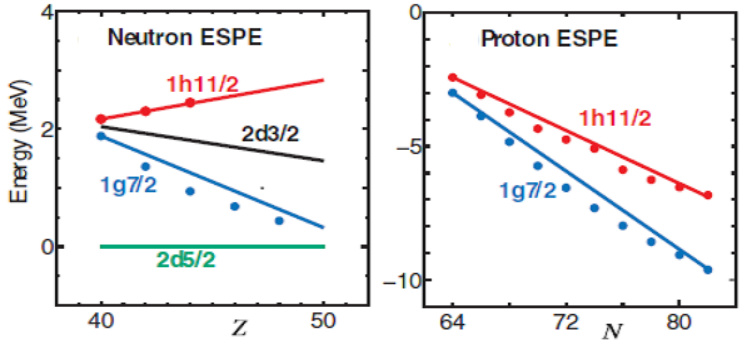
Prof. Shan-Gui Zhou's plenary talk
@ INPC2016, Australia

Tensor force and its effects

Tensor force is an important component of **NN interaction**

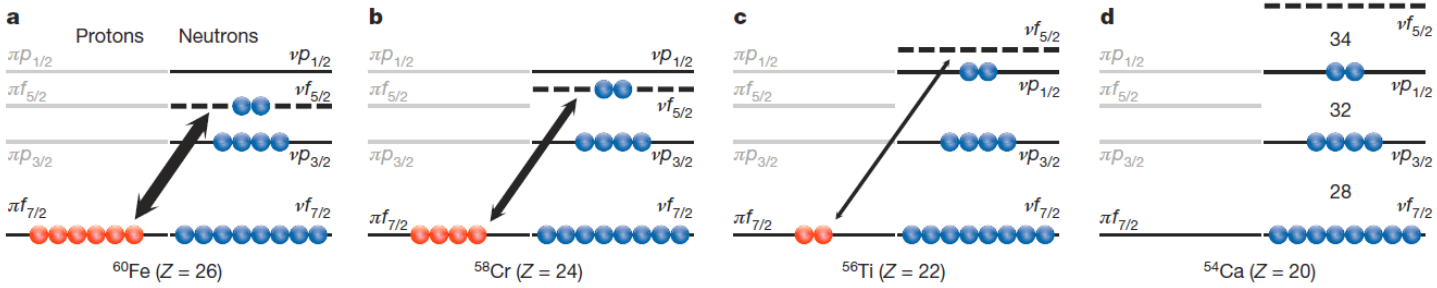
- Crucial for the **shell evolution** in exotic nuclei





Otsuka *et al.*, *PRL* **95**, 232502 (2005)

- Crucial for the **new magic numbers**

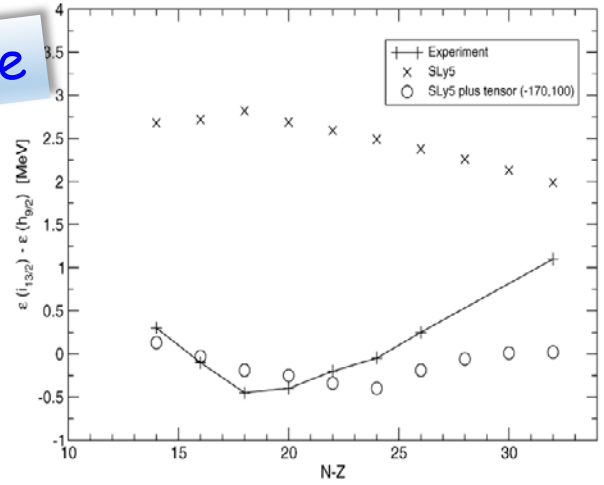


Steppenbeck *et al.*, *Nature* **502**, 207 (2013)

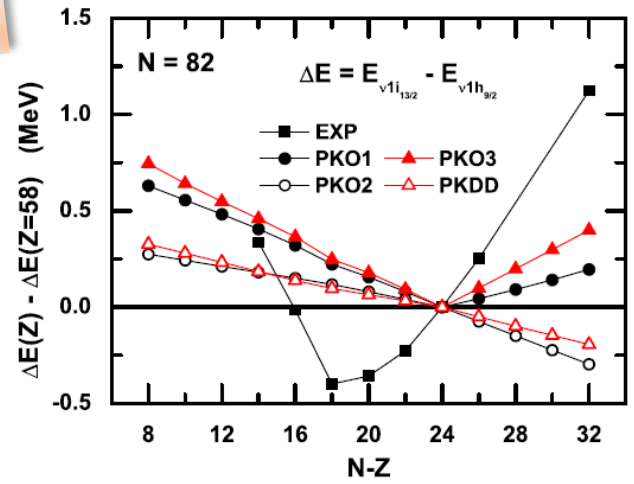
DFT and tensor effects

- **Shell evolution** ($N = 82$)

Skyrme



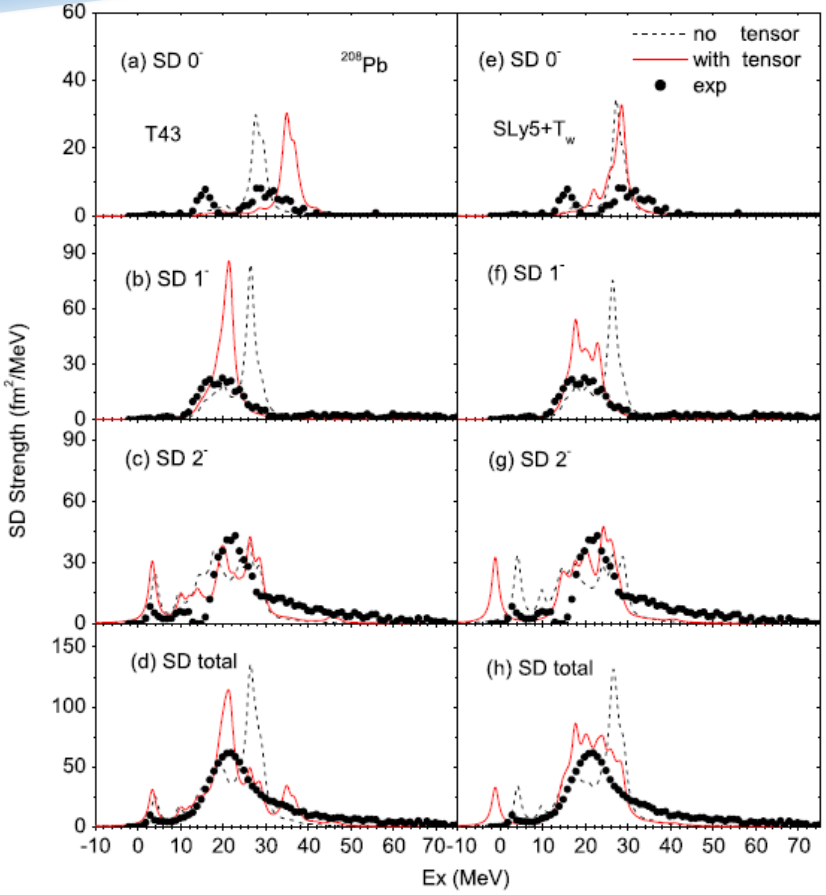
RHF



Colò, Sagawa, Fracasso, Bortignon, *PLB* **646**, 227 (2007)
Long, Sagawa, Meng, Giai, *EPL* **82**, 12001 (2008)
(exp) Schiffer et al., *PRL* **92**, 162501 (2004)

- **Giant resonances** (spin-dipole)

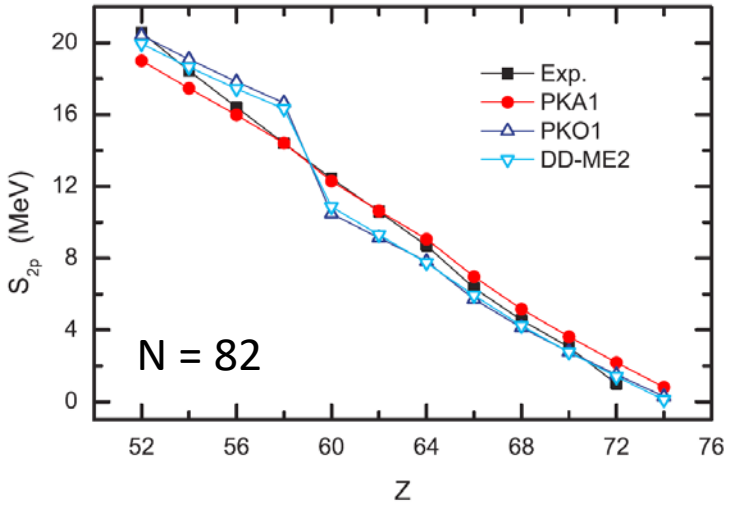
Skyrme



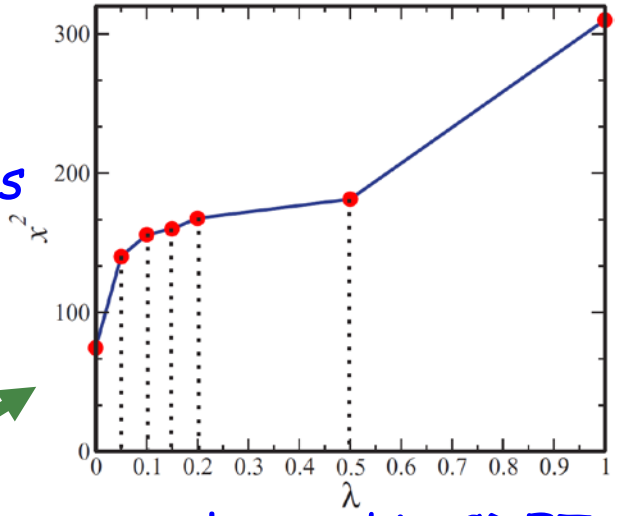
Bai, Zhang, Sagawa, Zhang, Colò, Xu, *PRL* **105**, 072501 (2010)
(exp) Wakasa et al., *PRC* **85**, 064606 (2012)

Tensor effects in relativistic DFT?

- Signals of tensor force in **relativistic DFT**? (nuclear mass)



some fingerprints



π meson (tensor) is not welcomed in CDFT

Long, Sagawa, Giai, Meng, *PRC* **76**, 034314 (2007)

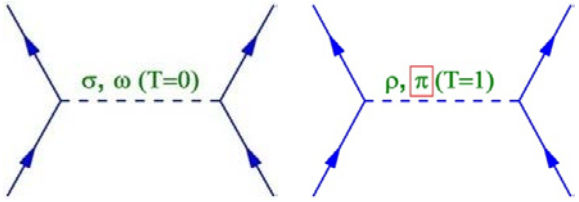
Lalazissis et al., *PRC* **80**, 041301(R) (2009)

- How to **identify** the tensor effects in relativistic DFT?
- Can we make **fair and quantitative comparison** with Skyrme, Gogny, etc.?
- What would be the proper ways to **determine the strengths** of tensor force?

Relativistic Hartree-Fock (RHF) theory

➢ **Lagrangian density**

Bouyssy *et al.*, *PRC* **36**. 380 (1987)
Long *et al.*, *PLB* **639**. 242 (2006)
HZL *et al.*, *PRL* **101**, 122502 (2008)



$$\mathscr{L} = \bar{\psi}\left(i\gamma_\mu\partial^\mu - M\right)\psi$$
$$+\frac{1}{2}\partial_\mu\sigma\partial^\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu + \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}_\mu\cdot\vec{\rho}^\mu - \frac{1}{4}\vec{R}_{\mu\nu}\cdot\vec{R}^{\mu\nu} + \frac{1}{2}\partial_\mu\vec{\pi}\cdot\partial^\mu\vec{\pi} - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$
$$-\bar{\psi}\left[g_\sigma\sigma + g_\omega\gamma^\mu\omega_\mu + g_\rho\gamma^\mu\vec{\tau}\cdot\vec{\rho}_\mu - \frac{f_\rho}{2M}\sigma^{\mu\nu}\vec{\tau}\cdot\partial_\nu\vec{\rho}_\mu + \frac{f_\pi}{m_\pi}\gamma_5\gamma^\mu\vec{\tau}\cdot\partial_\mu\vec{\pi} + e\gamma^\mu\frac{1-\tau_3}{2}A_\mu\right]\psi,$$

➢ **Hamiltonian**

$$H = \int d^3x\,\bar{\psi}(x)[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M]\psi(x) + \frac{1}{2}\sum_\phi\iint d^3x\,d^4y\,\bar{\psi}(x)\bar{\psi}(y)\Gamma_\phi(x,y)D_\phi(x,y)\psi(y)\psi(x)$$

interaction vertices **propagators**

According to interaction vertices, we have

σ-S, ω-V, ρ-V, ρ-T, ρ-VT, and π-PV couplings

Caution: **T** here indicates Dirac matrix $\boldsymbol{\sigma^{\mu\nu}}$, not the "tensor force"

- Their leading-order terms contain the **tensor force**. Sagawa & Colò, *PPNP* **76**, 76 (2014)
- **How about the next-to-the-leading-order terms? Are they important?**

Non-relativistic reduction

- Relativistic meson-exchange two-body interactions

$$\hat{V}_\phi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \gamma_0(\boldsymbol{r}_1)\gamma_0(\boldsymbol{r}_2)\Gamma_\phi(\boldsymbol{r}_1,\boldsymbol{r}_2)D_\phi(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

- Two-body interaction matrix elements

$$V_{\phi,\alpha\beta\gamma\delta} = \langle\varphi_\alpha\varphi_\beta|\hat{V}_\phi|\varphi_\gamma\varphi_\delta\rangle = \iint d\boldsymbol{r}_1\, d\boldsymbol{r}_2\, \varphi^\dagger_\alpha(\boldsymbol{r}_1)\varphi^\dagger_\beta(\boldsymbol{r}_2)\hat{V}_\phi(\boldsymbol{r}_1,\boldsymbol{r}_2)\varphi_\gamma(\boldsymbol{r}_1)\varphi_\delta(\boldsymbol{r}_2)$$

- **Non-relativistic reduced two-body interactions**

$$V_{\phi,\alpha\beta\gamma\delta} = \langle\varphi_\alpha\varphi_\beta|\hat{\mathcal{V}}_\phi\Pi_+|\varphi_\gamma\varphi_\delta\rangle = \langle\xi_\alpha\xi_\beta|\hat{\mathcal{V}}_\phi|\xi_\gamma\xi_\delta\rangle$$

ξ: upper component
$\hat{\mathcal{V}}$ can be expanded in the **powers of 1/M**
(~ **Foldy-Wouthuysen method** for one-body problem)

Example: plane waves in finite-density systems

$$V_{\phi,abcd} = \bar{u}_{\boldsymbol{p}^*_a}(1)\bar{u}_{\boldsymbol{p}^*_b}(2)\frac{1}{m^2_\phi+\boldsymbol{q}^2}\Gamma_\phi(1,2)u_{\boldsymbol{p}^*_c}(1)u_{\boldsymbol{p}^*_d}(2)$$

with $$u_{\boldsymbol{p}^*_a} = \sqrt{\frac{M^*+\varepsilon^*_a}{2\varepsilon^*_a}}\begin{pmatrix} 1 \\ \frac{\boldsymbol{\sigma}\cdot\boldsymbol{p}^*_a}{M^*+\varepsilon^*_a}\end{pmatrix}$$

$$\boldsymbol{p}^* \equiv \boldsymbol{p} + \hat{\boldsymbol{p}}\Sigma_V(p)$$
$$M^*(p) \equiv M + \Sigma_S(p)$$
$$\varepsilon^*(p) \equiv \varepsilon(p) - \Sigma_0(p)$$

Non-relativistic reduced interactions

- Up to the $1/M^2$ order

$$S_{12} \equiv (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) - \frac{1}{3}(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)q^2$$

$$\begin{aligned}
\hat{\mathcal{V}}_{\sigma\text{-S}} = & -g_\sigma(1)g_\sigma(2)\frac{1}{m_\sigma^2+\boldsymbol{q}^2}\left[1-\frac{1}{4}\frac{4\boldsymbol{k}^2-\boldsymbol{q}^2-4i\boldsymbol{\sigma}_1\cdot(\boldsymbol{k}\times\boldsymbol{q})}{4M^*(1)M^*(1)}-\frac{1}{4}\frac{4\boldsymbol{k}'^2-\boldsymbol{q}^2-4i\boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k}')}{4M^*(2)M^*(2)}\right], \\
\hat{\mathcal{V}}_{\omega\text{-V}} = & +g_\omega(1)g_\omega(2)\frac{1}{m_\omega^2+\boldsymbol{q}^2}\left[1+\frac{1}{4}\frac{4\boldsymbol{k}^2-\boldsymbol{q}^2-4i\boldsymbol{\sigma}_1\cdot(\boldsymbol{k}\times\boldsymbol{q})}{4M^*(1)M^*(1)}+\frac{1}{4}\frac{4\boldsymbol{k}'^2-\boldsymbol{q}^2-4i\boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k}')}{4M^*(2)M^*(2)}\right] \\
& -\frac{g_\omega(1)g_\omega(2)}{4M^*(1)M^*(2)}\frac{1}{m_\omega^2+\boldsymbol{q}^2}\left[4\boldsymbol{k}\boldsymbol{k}'+2i\boldsymbol{\sigma}_1\cdot(\boldsymbol{q}\times\boldsymbol{k}')-2i\boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k})+\frac{2}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\boldsymbol{q}^2-S_{12}\right], \\
\hat{\mathcal{V}}_{\pi\text{-PV}} = & -\vec{\tau}(1)\cdot\vec{\tau}(2)\frac{f_\pi(1)f_\pi(2)}{m_\pi^2}\frac{1}{m_\pi^2+\boldsymbol{q}^2}\left[S_{12}+\frac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\boldsymbol{q}^2\right], \\
\hat{\mathcal{V}}_{\rho\text{-T}} = & +\vec{\tau}(1)\cdot\vec{\tau}(2)\frac{f_\rho(1)f_\rho(2)}{4M^2}\frac{1}{m_\rho^2+\boldsymbol{q}^2}\left[S_{12}-\frac{2}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\boldsymbol{q}^2\right], \\
\hat{\mathcal{V}}_{\rho\text{-VT}} = & +\vec{\tau}(1)\cdot\vec{\tau}(2)\frac{f_\rho(1)g_\rho(2)}{4MM^*(1)}\frac{1}{m_\rho^2+\boldsymbol{q}^2}\left[-\boldsymbol{q}^2+2i\boldsymbol{\sigma}_1\cdot(\boldsymbol{q}\times\boldsymbol{k})\right] \\
& +\vec{\tau}(1)\cdot\vec{\tau}(2)\frac{f_\rho(1)g_\rho(2)}{4MM^*(2)}\frac{1}{m_\rho^2+\boldsymbol{q}^2}\left[-2i\boldsymbol{\sigma}_1\cdot(\boldsymbol{q}\times\boldsymbol{k}')-\frac{2}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\boldsymbol{q}^2+S_{12}\right] \\
& +\vec{\tau}(1)\cdot\vec{\tau}(2)\frac{g_\rho(1)f_\rho(2)}{4MM^*(2)}\frac{1}{m_\rho^2+\boldsymbol{q}^2}\left[-\boldsymbol{q}^2-2i\boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k}')\right] \\
& +\vec{\tau}(1)\cdot\vec{\tau}(2)\frac{g_\rho(1)f_\rho(2)}{4MM^*(1)}\frac{1}{m_\rho^2+\boldsymbol{q}^2}\left[+2i\boldsymbol{\sigma}_2\cdot(\boldsymbol{q}\times\boldsymbol{k})-\frac{2}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\boldsymbol{q}^2+S_{12}\right].
\end{aligned}$$

Finite density

Formalism is in agreement with **Bonn interaction**: Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989)

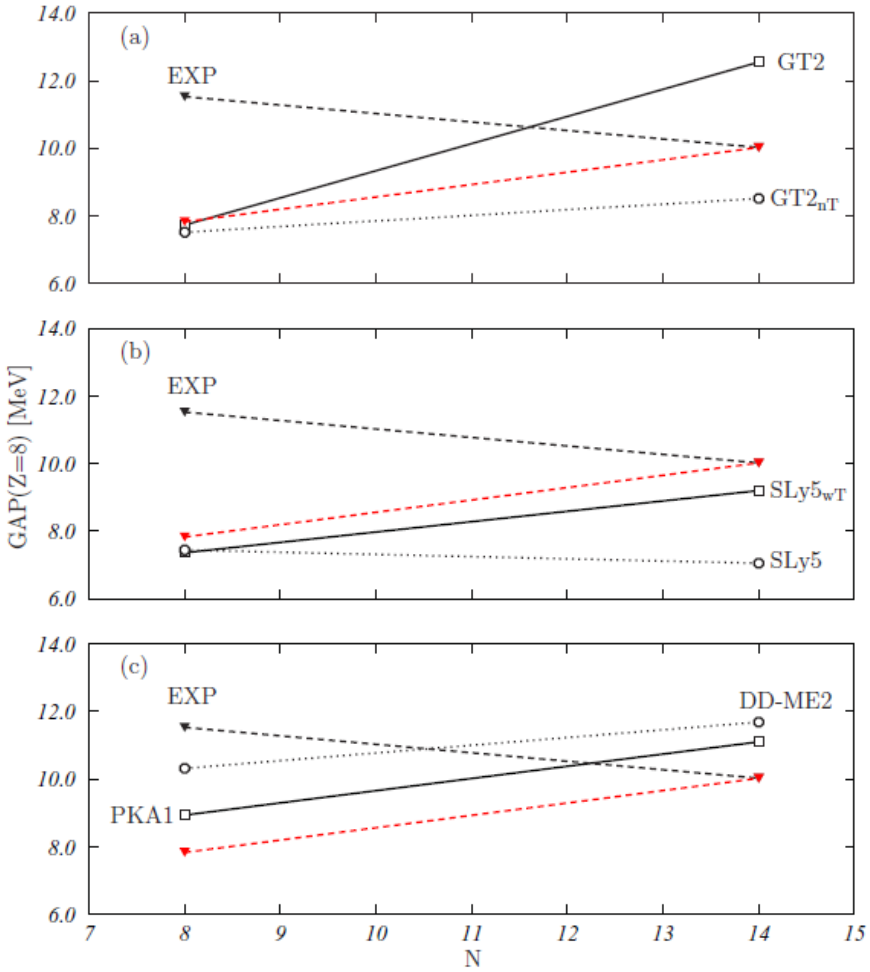
Tensor effects on shell evolution

PHYSICAL REVIEW C **81**, 064327 (2010)

Tensor effects in shell evolution at $Z, N = 8, 20$, and 28 using nonrelativistic and relativistic mean-field theory

M. Moreno-Torres,[1] M. Grasso,[2] H. Liang,[2,3] V. De Donno,[4] M. Anguiano,[1] and N. Van Giai[2]

Skyrme *vs* Gogny *vs* RHF



Gogny:

GT2 *vs* $GT2_{nT}$

Tensor effect

~ 4 MeV

Skyrme:

$SLy5_{wT}$ *vs* SLy5

Tensor effect

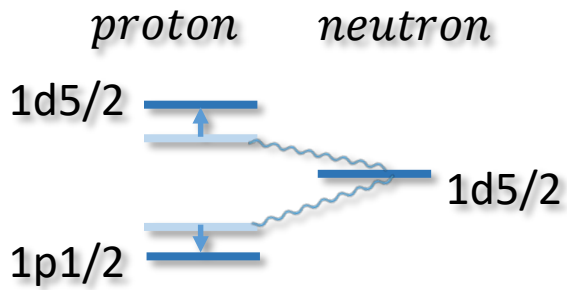
~ 2.5 MeV

RHF:

PKA1 *vs* DD-ME2

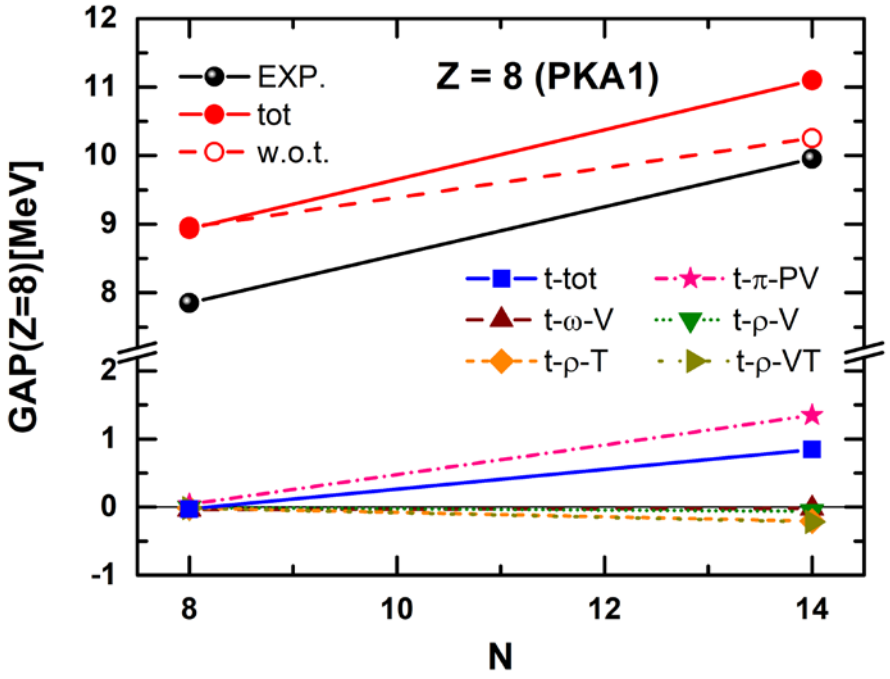
Tensor effect

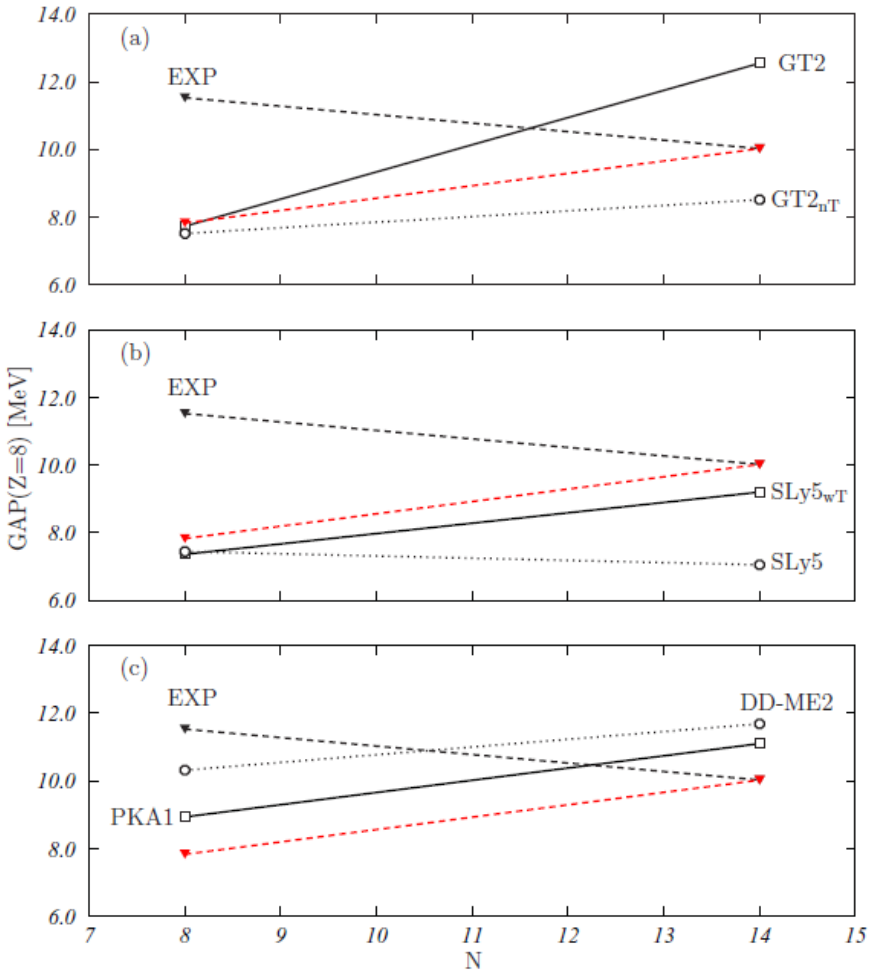
? MeV



From ^{16}O to ^{22}O

Tenser effects on gap Z=8





PKA1 *vs* $PKA1_{nT}$

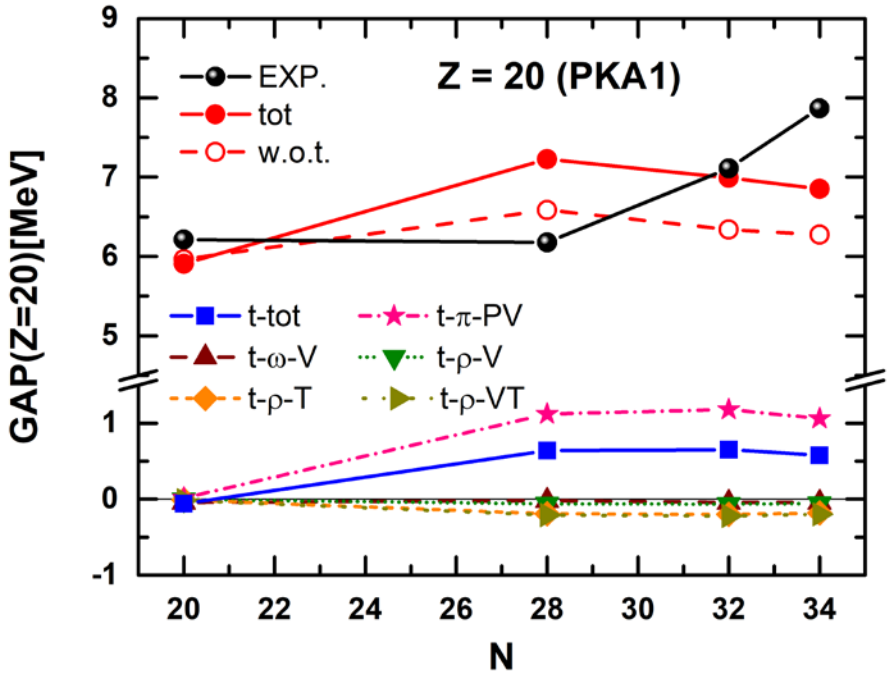
Tensor effect **~ 1 MeV**

first fair comparison

- The **same behavior** of tensor force but **weaker** than Skyrme and Gogny

Wang, Zhao, HZL, Long, *PRC* **98**, 034313 (2018)

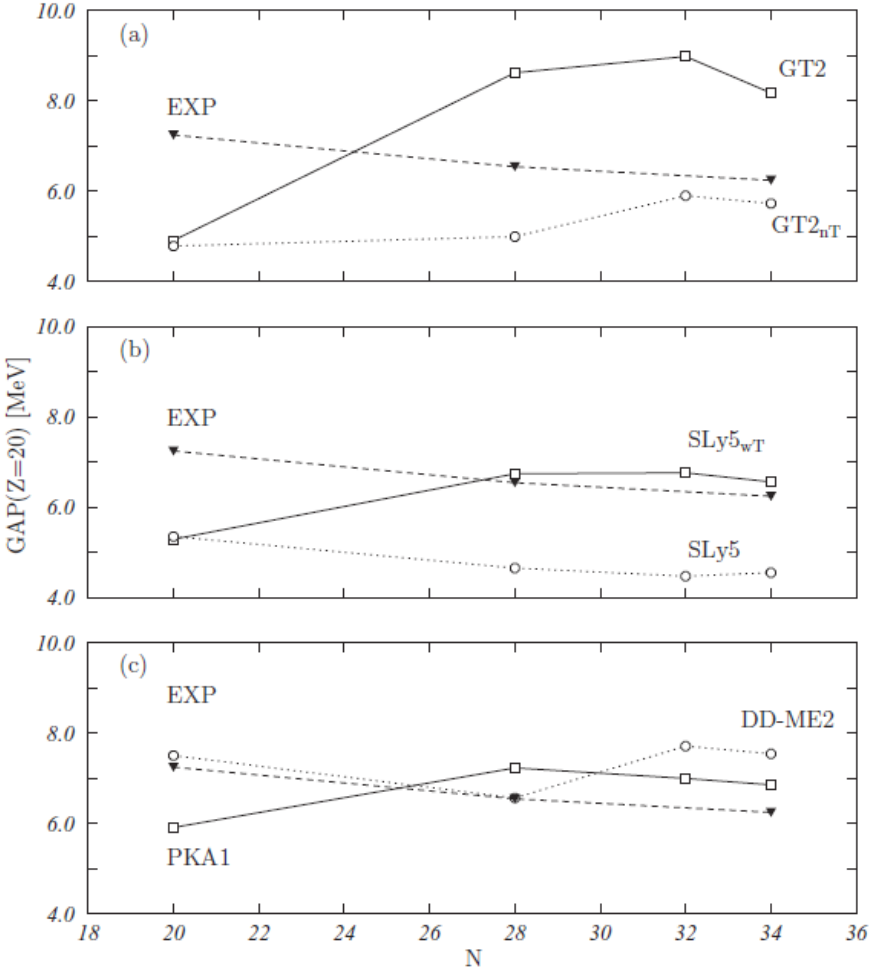
Tenser effects on gap Z=20



Wang, Zhao, HZL, Long, *PRC* **98**, 034313 (2018)

- **Quite similar behavior** as Skyrme
- But **too weak?**

What are proper benchmarks?

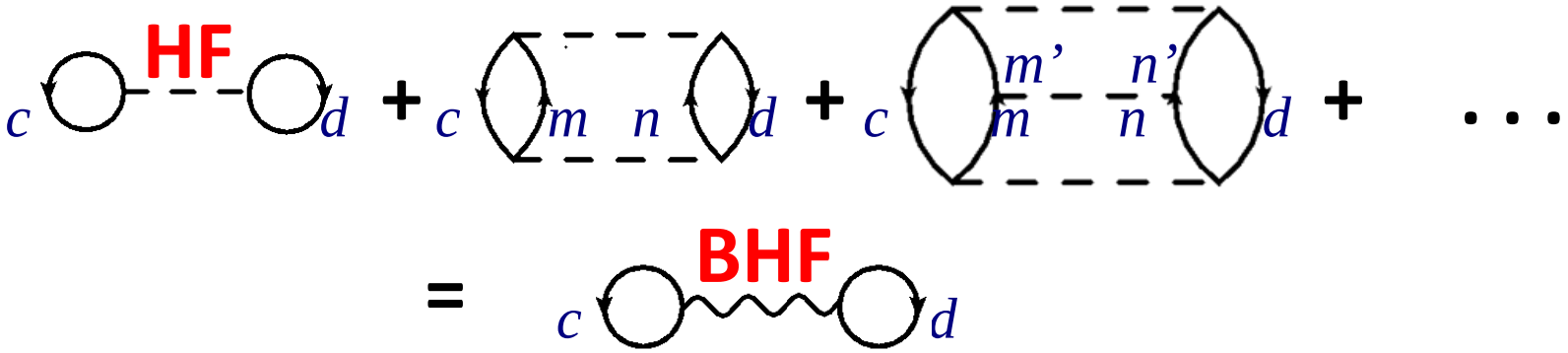


Moreno-Torres *et al.*, *PRC* **81**. 064327 (2010)

Ab initio for relativistic DFT

- Brueckner-Hartree-Fock theory (*ladder diagrams to all order*)

(with exchange terms as well)



- Bethe-Goldstone equation → **finite nuclei**

$$\langle ab|G(W)|cd\rangle = \langle ab|V|cd\rangle + \sum_{mn}\langle ab|V|mn\rangle \frac{Q(m,n)}{W-\varepsilon_m-\varepsilon_n}\langle mn|G(W)|cd\rangle$$

where the starting energy $W = \varepsilon_c + \varepsilon_d$

For the first time, **Bethe-Goldstone equation** is solved **self-consistently**

- in the **rest** frame
- in pure **relativistic** scheme

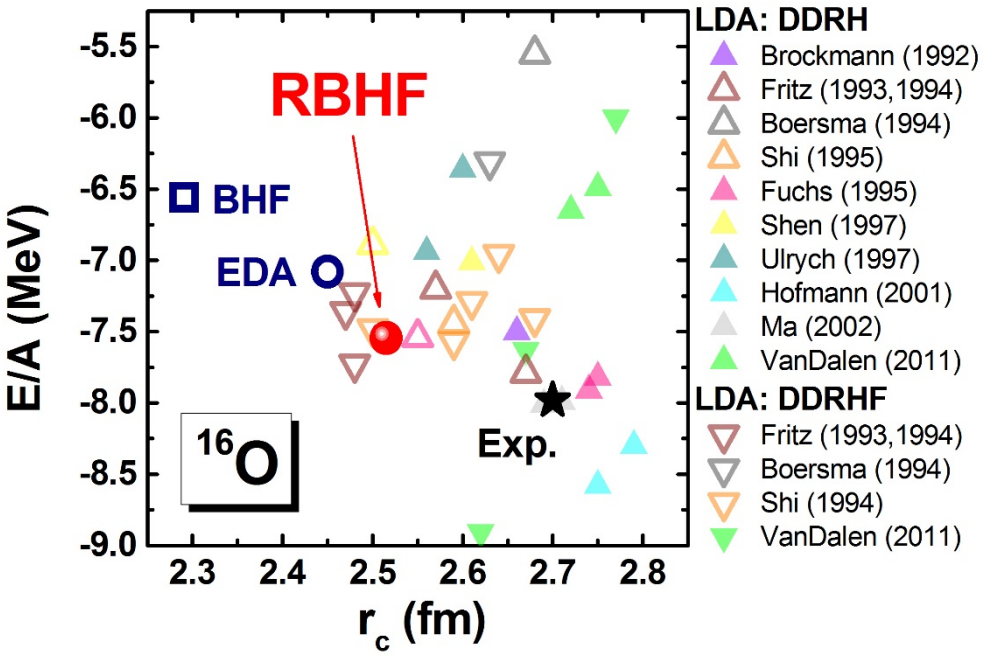
PKU scholarship & RIKEN IPA project

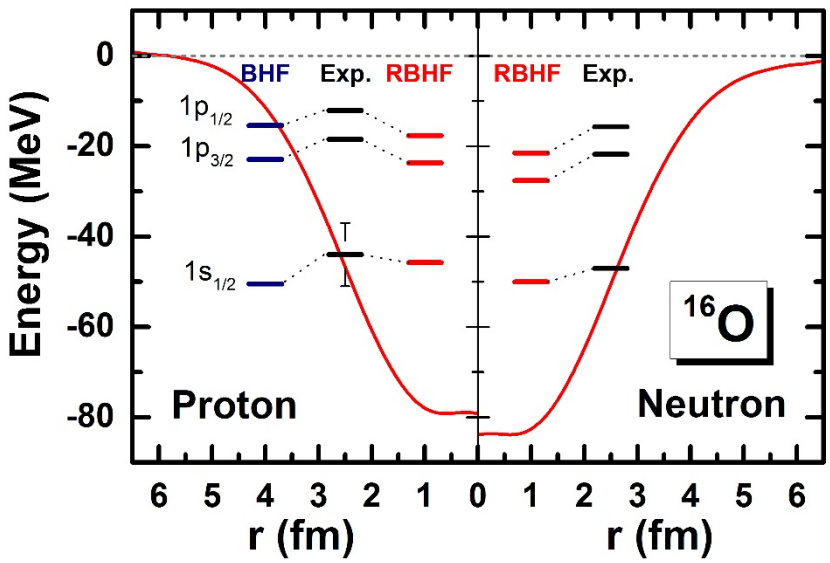
Shen, Hu, HZL, Meng, Ring, Zhang, *Chin. Phys. Lett.* **33**, 102103 (2016)

Shen, HZL, Meng, Ring, Zhang, *Phys. Rev. C* **96**, 014316 (2017)

Relativistic BHF for finite nuclei

- Relativistic BHF calculations for ^{16}O with Bonn A interaction





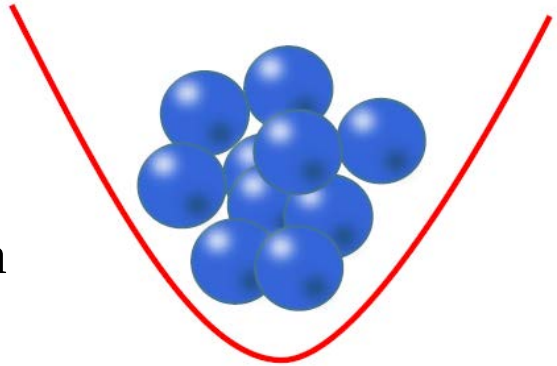
EDA = effective density approximation [Müther(1990)]
LDA = local density approximation

Shen, Hu, HZL, Meng, Ring, Zhang, *Chin. Phys. Lett.* **33**, 102103 (2016)

- a first *ab initio* calculations for finite nuclei in **relativistic** scheme
- **Spin-orbit** splitting is reproduced well from the bare interaction
- benchmark for various LDA calculations

Neutron drops

Neutron drop is a multi-neutron system confined in an external field.



Why neutron drops?

- Simple, can be accessed by many *ab initio* methods
- An ideal environment for studying neutron rich system

Pudliner et al., *PRL* **76**, 2416 (1996)
Gandolfi, Carlson, Pieper, *PRL* **106**, 012501 (2011)
Maris et al., *PRC* **87**, 054318 (2013)
Potter et al., *PLB* **739**, 445 (2014)
Zhao & Gandolfi, *PRC* **94**, 041302(R) (2016)
Shen, Colò , Roca-Maza, *PRC* **99**, 034322 (2019)
……

Relativistic Brueckner-Hartree-Fock (RBHF) theory for neutron drops

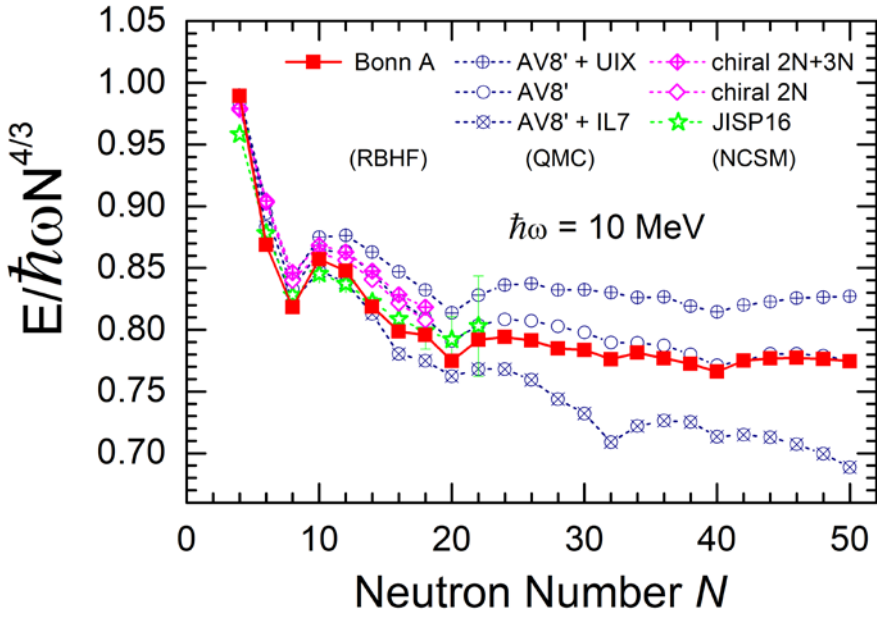
- Neither RBHF nor CDFT includes **beyond-mean-field effects**

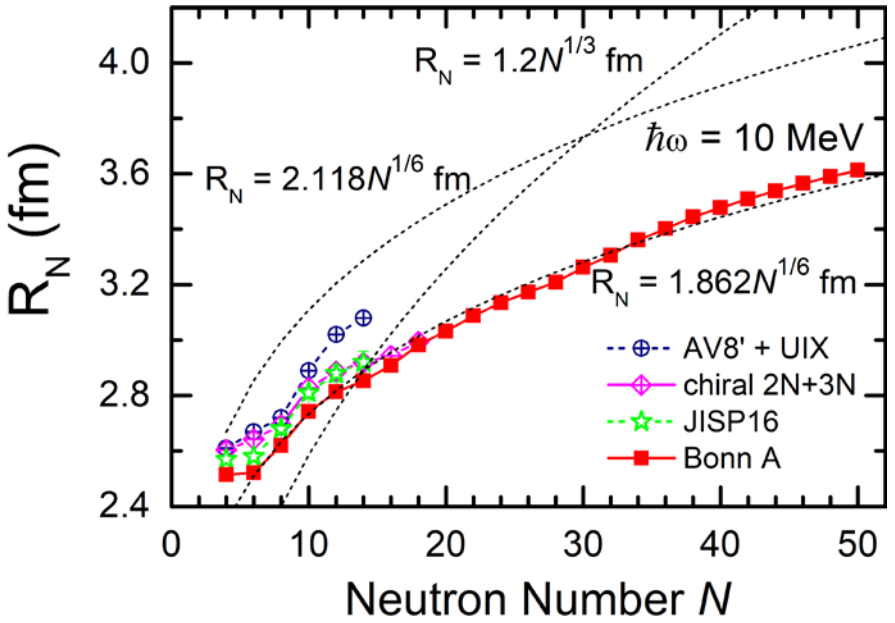
  ➔ **it is a fair comparison!**

Shen, Hu, HZL, Meng, Ring, Zhang, *CPL* **33**, 102103 (2016)
Shen, HZL, Meng, Ring, Zhang, *PRC* **96**, 014316 (2017)
Shen, HZL, Meng, Ring, Zhang, *PLB* **778**, 344 (2018)
Shen, HZL, Meng, Ring, Zhang, *PRC* **97**, 054312 (2018)
Shen, HZL, Meng, Ring, Zhang, *PLB* **781**, 227 (2018)

Energies and radii

- Relativistic BHF calculations for neutron drops with Bonn A interaction



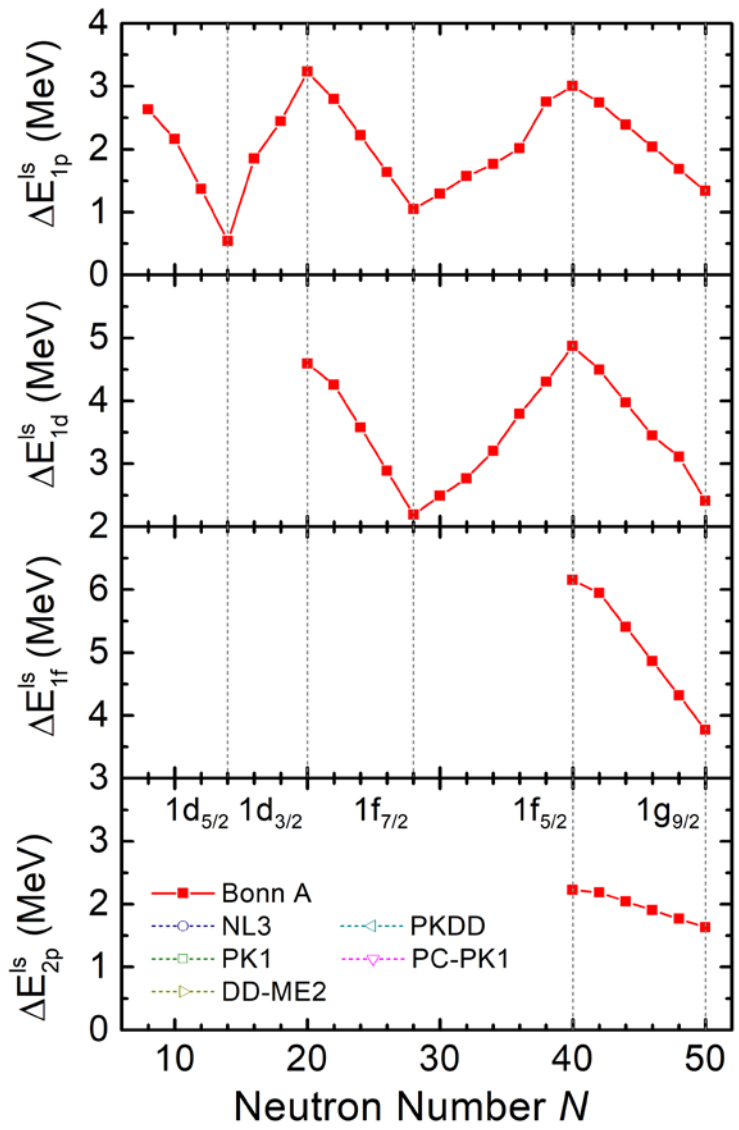


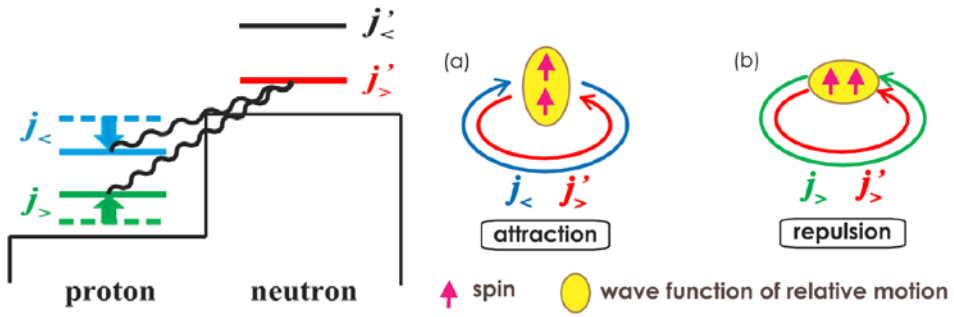
Gandolfi, Carlson, Pieper, *PRL* **106**, 012501 (2011)
Maris et al., *PRC* **87**, 054318 (2013)
Potter et al., *PLB* **739**, 445 (2014)

Shen, HZL, Meng, Ring, Zhang,
Phys. Lett. B **778**, 344 (2018)
Phys. Lett. B **781**, 227 (2018)
Phys. Rev. C **97**, 054312 (2018)

- Energies ***E*** and radii R_N are consistent with JISP16 or AV8'.
- R_N follows the $N^{1/6}$ law.

Spin-orbit splitting (RBHF)





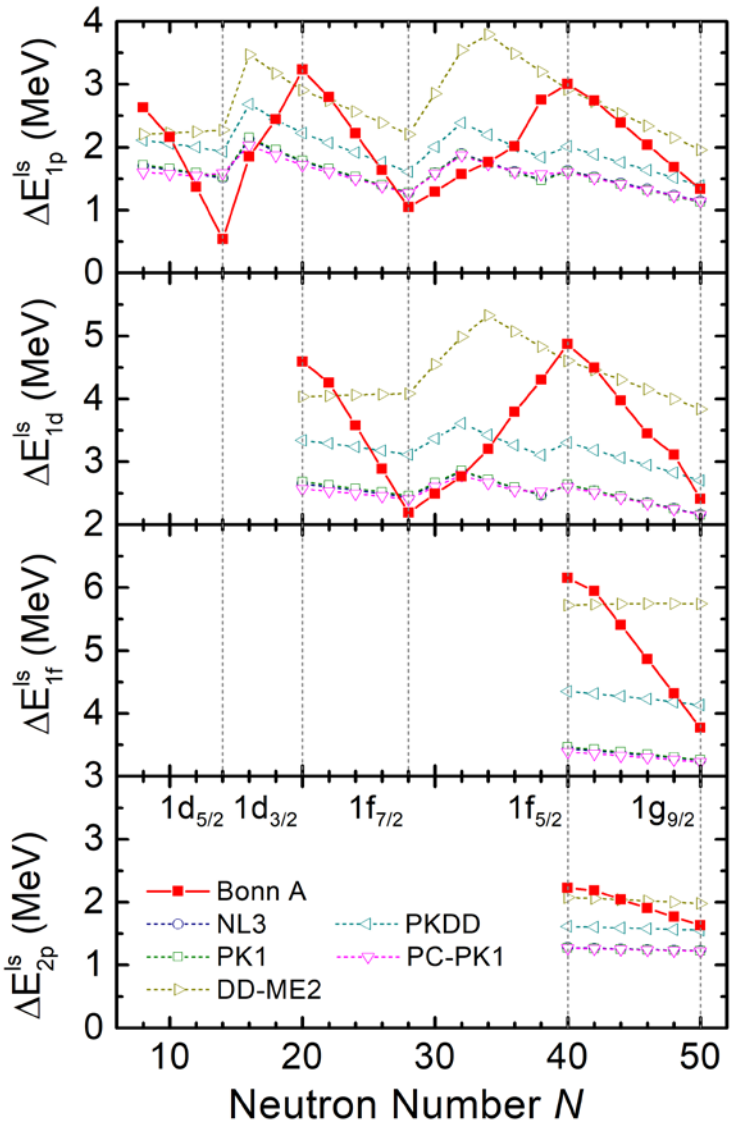
Otsuka *et al.*, *Phys. Rev. Lett.* **95**, 232502 (2005)

Meta-data for tensor effect

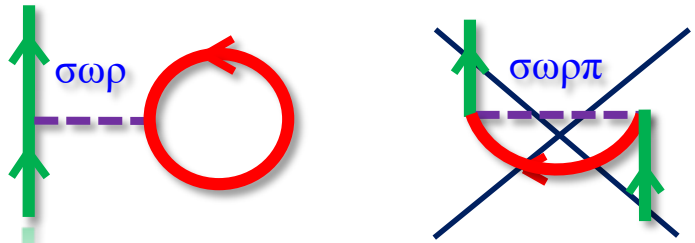
- The SO splitting **decreases** as the spin-up $j_> = l + 1/2$ orbitals are filled, while the SO splitting **increases** as the spin-down $j_< = l + 1/2$ orbitals are filled.

Shen, HZL, Meng, Ring, Zhang, *PLB* **778**, 344 (2018); *PLB* **781**, 227 (2018); *PRC* **97**, 054312 (2018)

Spin-orbit splitting (RMF)



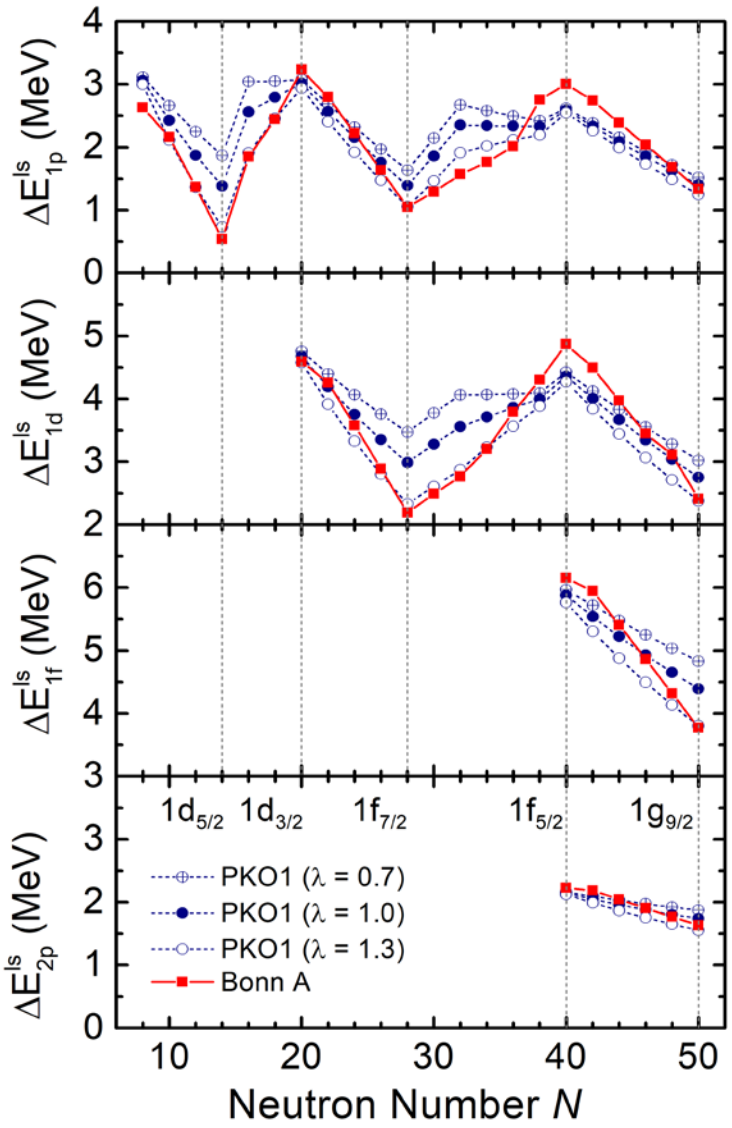
- Comparison with the **phenomenological** relativistic mean-field (**RMF**) energy density functionals (EDF).



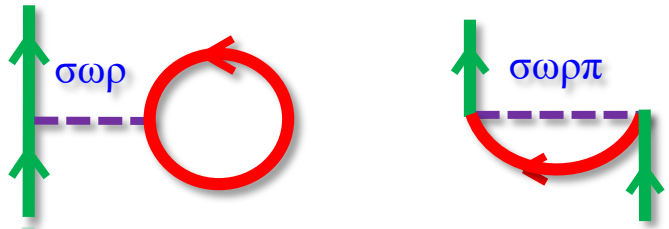
- **None of them can reproduce this tensor behavior!**

Shen, HZL, Meng, Ring, Zhang, *PLB* **778**, 344 (2018); *PLB* **781**, 227 (2018); *PRC* **97**, 054312 (2018)

Spin-orbit splitting (RHF)



- Comparison with the **phenomenological** relativistic Hartree-Fock (**RHF**) energy density functionals (EDF).

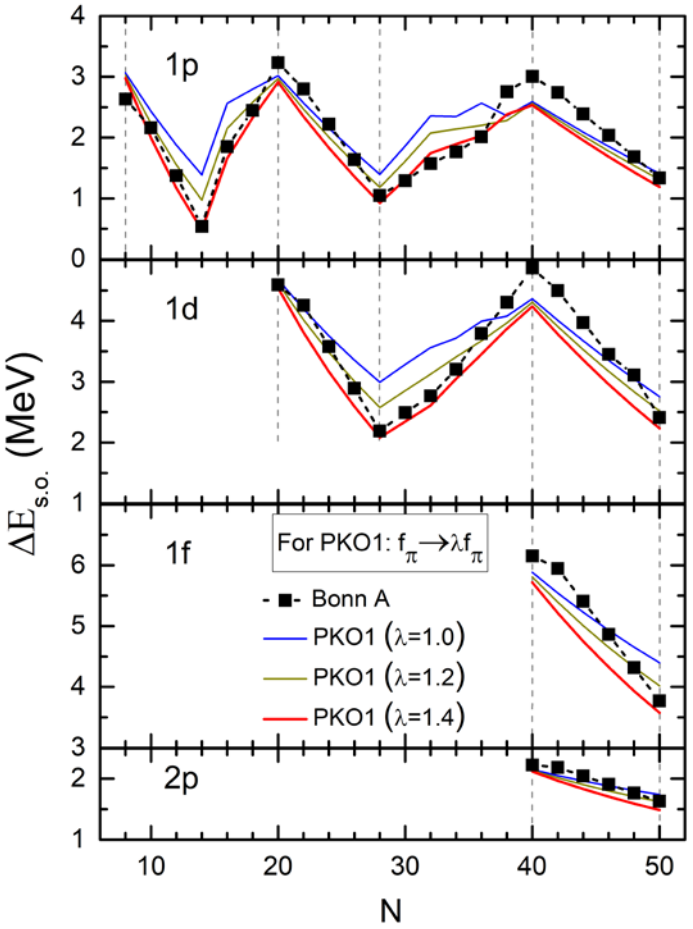


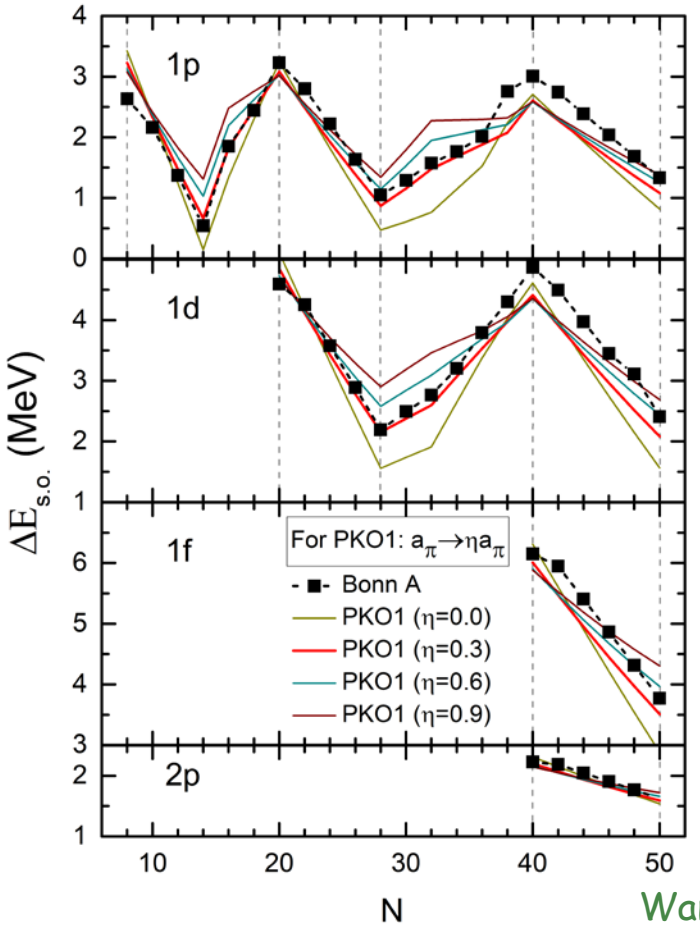
- **RHF** (PKO1) shows a very similar pattern, but with **stronger tensor strengths**
- Neither RBHF nor CDFT includes **beyond-mean-field effects**

  ➔ **it is a fair comparison!**

Shen, HZL, Meng, Ring, Zhang, *PLB* **778**, 344 (2018); *PLB* **781**, 227 (2018); *PRC* **97**, 054312 (2018)

Exploration of strength of tensor force





$$f_\pi(\xi) = f_\pi(0)e^{-a_\pi \xi}$$

$$\xi \equiv \rho_b/\rho_{\mathrm{sat.}}$$

Wang, PhD thesis (2018)

- Increasing the strengths of tensor force: $f_\pi \rightarrow 1.4 f_\pi$ or $a_\pi \rightarrow 0.3 a_\pi$
- Small a_π → "Tensor renormalization persistency"

cf. Tsunoda *et al.*, *PRC*, **84**, 044322 (2011)

Summary

- **A first quantitative analysis of tensor effects** in the relativistic Hartree-Fock theory
  - ✓ It allows **fair and direct comparisons** with Skyrme, Gogny, etc.
  - ✓ We have investigated the tensor effects on shell evolutions, spin-orbit splitting, spin-isospin resonances, etc. ➔ The strengths of tensor force in present EDFs **seem too weak**.
- **A first relativistic *ab initio* calculation for finite nuclei** by the relativistic Brueckner-Hartree-Fock (RBHF) theory
  - ✓ The binding energies and radii of ^{16}O are reasonable
  - ✓ **Spin-orbit splitting** is well reproduced ➔ bare NN interaction together with relativistic scheme
- **Remarkable tensor effects on spin-orbit splitting in neutron drops**
  - ✓ **Important guideline** for phenomenological EDF

Contents

Fundamentals of Density Functional Theory

- Interesting viewpoints on **DFT**
- Hohenberg-Kohn (**HK**) theorem
- Kohn-Sham (**KS**) scheme
- *Discussion*: some open issues

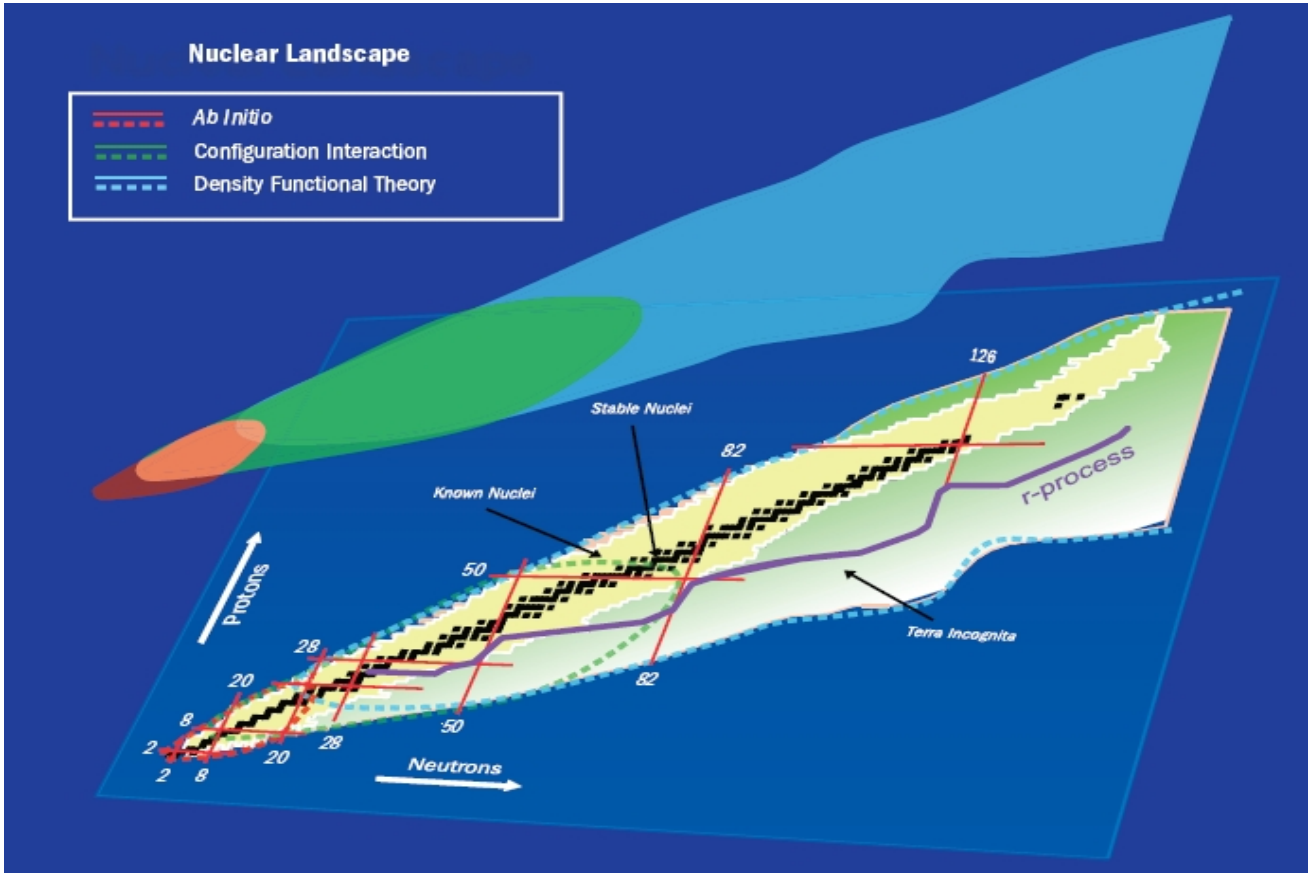
Nuclear DFT and applications

- Covariant Density Functional Theory (**CDFT**)
- *Application*: Nuclear tensor force and its effects

Connections to Quantum Field Theory

- Energy density functional and effective action in **QFT**
- Functional Renormalization Group (**FRG**)
- *Application*: φ^4-theory in zero dimension

State-of-the-art nuclear methodologies

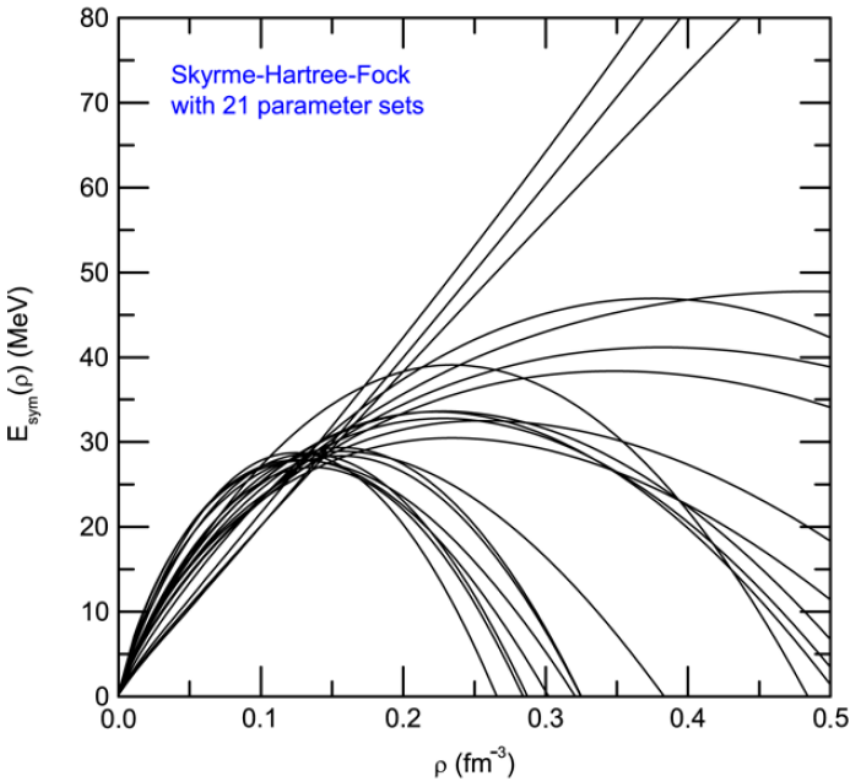


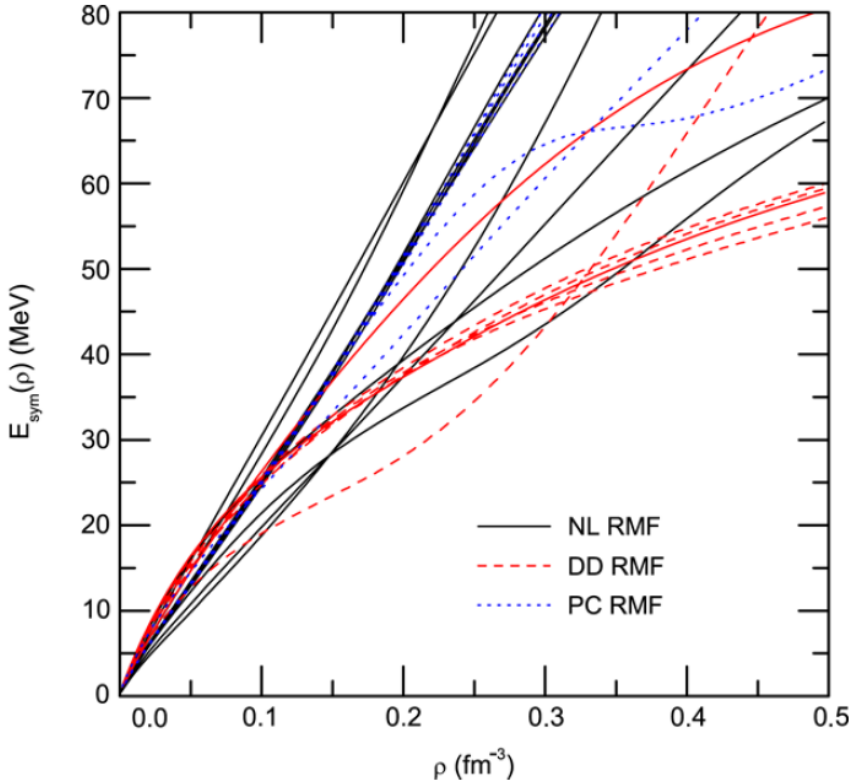
http://www.unedf.org/

- Density functional theory (DFT) aims at understanding both ground-state and excited-state properties of thousands of nuclei in a consistent and predictive way.

Phenomenological energy density functionals

- ***Predictions*** **of phenomenological EDF (10 years ago)**





Li, Chen, Ko, *Phys. Rep.* **464**, 113 (2008)

Toward *ab initio* DFT

Progress in Particle and Nuclear Physics 64 (2010) 120–168

DFT as Legendre transform via **path integrals** for **effective actions**

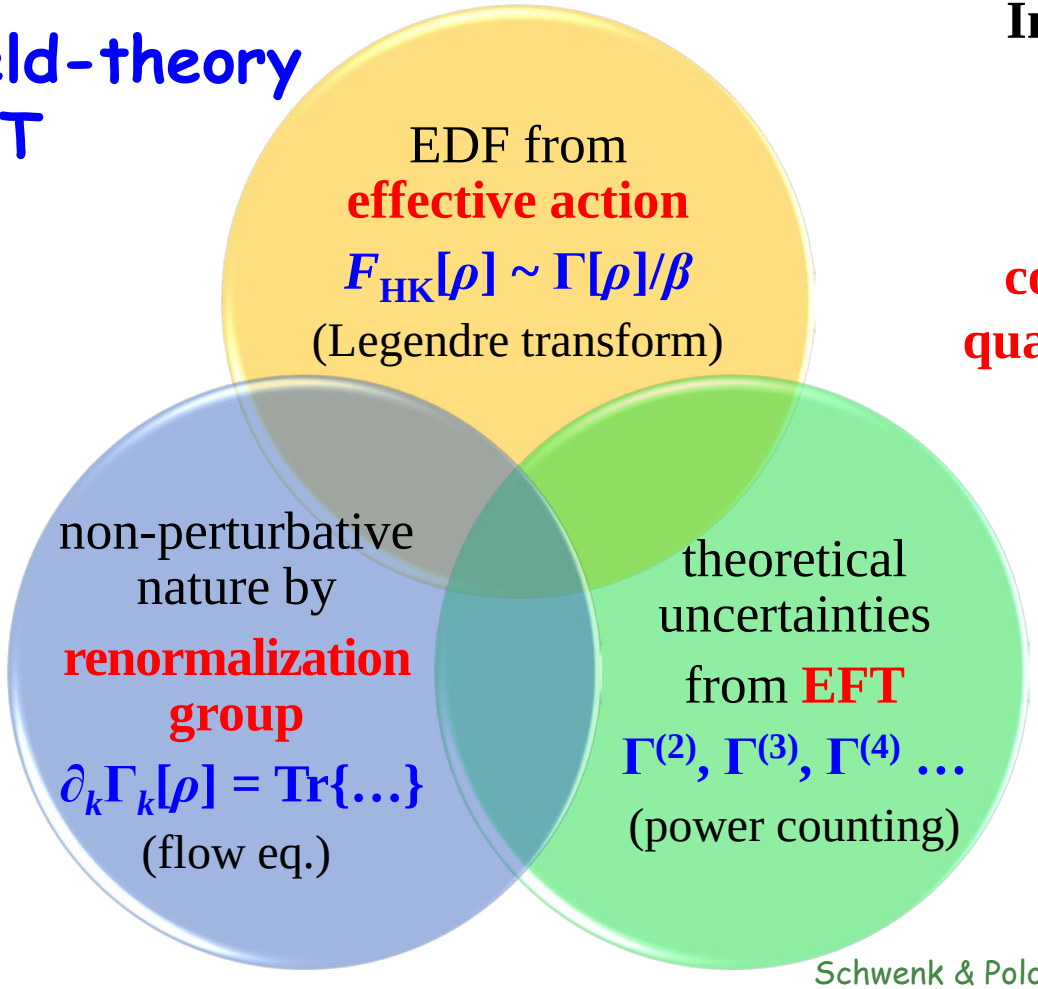
- Effective actions are the **natural theoretical framework** for Legendre transforms, which is the **underlying basis** for DFT.
- Path integral construction of DFT is **transparent**.
- Path integral effective actions are particularly suited for **symmetry breaking**.
- Connections to **EFT** and **power counting** can be more accessible.
- Path integral formulation puts the DFT construction in a **broader perspective**.
- Path integral formulation can suggest **different kinds of non-perturbative approximations**.
- ……

Various paths to a DFT effective action

- The auxiliary field (Hubbard-Stratonovich) method
- The inversion method
- The RG approach

A dream for next-generation DFT

quantum-field-theory oriented DFT



Interdisciplinary:
(lattice) QCD
hadron
cold atom
condensed matter
quantum chemistry
……

also cf.
Schwenk & Polonyi, arXiv:0403011 [nucl-th]
Kutzelnigg, JMS 768, 163 (2006)
Drut, Furnstahl, Platter, PPNP 64, 120 (2010)
Braun, JPG 39, 033001 (2012)
Metzner et al., RMP 84, 299 (2012)
Drews & Weise, PPNP 93, 69 (2017)
……

Density Functional Theory

The aim of density functional theory (DFT) is

- to reduce the many-body quantum mechanical problem formulated in terms of N-particle wave functions Ψ to the one-particle level with the local density distribution $\rho(\mathbf{x})$.

Hohenberg-Kohn theorem [*Phys. Rev.* **136**, B864 (1964)]

- ✓ There exist **a universal density functional** $F_{\mathrm{HK}}[\rho(\mathbf{x})]$.
- ✓ The ground-state energy E_{gs} attains **its minimum** value when the density $\rho(\mathbf{x})$ has its correct ground-state value.

HK variational principle

$$E_U = \inf_{\rho} \left\{ F_{\mathrm{HK}}[\rho(\mathbf{x})] + \int \mathrm{d}^d\mathbf{x}\, U(\mathbf{x})\rho(\mathbf{x}) \right\}$$

Goal: $F_{\mathrm{HK}}[\rho]$

Where $F_{\mathrm{HK}}[\rho(\mathbf{x})] = \min_{\Psi_\rho} \langle \Psi_\rho | \hat{T} + \hat{V} | \Psi_\rho \rangle$ is **a universal functional**, which is valid for any number of particles N and for any external field $U(\mathbf{x})$.

EDF from effective action

Strategy: $F_{\mathrm{HK}}[\rho]$ ← $\Gamma[\rho]$ ← partition function ← path integral

- **Classical action** in Euclidean space

$$S_{\mathrm{E}}[\psi^\dagger,\psi] = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, \psi^\dagger(\tau,\mathbf{x}) \left(\frac{\partial}{\partial\tau} - \frac{\nabla^2}{2M} + U(\mathbf{x}) \right) \psi(\tau,\mathbf{x})$$
$$+\frac{1}{2}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}_1 \mathrm{d}^d\mathbf{x}_2\, \psi^\dagger(\tau,\mathbf{x}_1)\psi^\dagger(\tau,\mathbf{x}_2)V(\mathbf{x}_1,\mathbf{x}_2)\psi(\tau,\mathbf{x}_2)\psi(\tau,\mathbf{x}_1)$$

  where $U(x)$ is one-body potential and $V(x_1, x_2)$ is two-body interaction.

- **Partition function** in two-particle point-irreducible (**2PPI**) scheme

$$Z[J] = \int \mathfrak{D}\psi^\dagger\, \mathfrak{D}\psi\, \exp\left[-S[\psi^\dagger,\psi] + \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, J(\tau,\mathbf{x})\psi^\dagger(\tau,\mathbf{x})\psi(\tau,\mathbf{x}) \right]$$

  external source J couples $\psi^\dagger\psi$ at the same space-time.

- **Thermodynamic potential** / generating function / Schwinger function

$$W[J] = \ln Z[J]$$

$$E_{\mathrm{gs}} = \lim_{\beta\to\infty} -\frac{1}{\beta} W$$

Connection to Hohenberg-Kohn theorem

- **Local density**

$$\rho(\tau,\mathbf{x}) = \langle \psi^\dagger(\tau,\mathbf{x})\psi(\tau,\mathbf{x})\rangle = \frac{\delta W[J]}{\delta J(\tau,\mathbf{x})}$$

$$E_{\rm gs}[\rho] = \lim_{\beta\to\infty}\frac{1}{\beta}\Gamma[\rho]|_{J\to 0}$$

- **Effective action ← Legendre transform** of ***W*** with respect to ***J***

$$\Gamma[\rho] = \sup_{\{J\}}\left\{-W[J] + \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, J(\tau,\mathbf{x})\rho(\tau,\mathbf{x})\right\}$$

✓ The **universality** of the **Hohenberg-Kohn functional** $F_{\rm HK}[\rho]$ follows from the fact that the background ***U*** potential can be absorbed into the source terms ***J*** by a simple shift ***J*** → ***J*** – ***U***.

Second **Legendre transform** → **HK theorem**

$$E_U = \inf_\rho\left\{F_{\rm HK}[\rho(\mathbf{x})] + \int \mathrm{d}^d\mathbf{x}\, U(\mathbf{x})\rho(\mathbf{x})\right\}$$

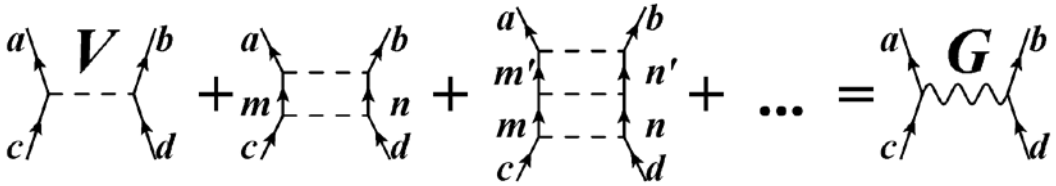
proof

$$\begin{aligned}\Gamma_U[\rho] &= -W_U[J] + \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, J(\mathbf{x})\rho(\mathbf{x}) \\ &= -W_0[J-U] + \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, [J(\mathbf{x})-U(\mathbf{x})]\,\rho(\mathbf{x}) + \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, U(\mathbf{x})\rho(\mathbf{x}) \\ &= \Gamma_0[\rho] + \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x}\, U(\mathbf{x})\rho(\mathbf{x})\end{aligned}$$

Non-perturbative nature of interaction

- **Lippmann-Schwinger eq. / Bethe-Goldstone eq. / Brueckner theory**
  Brueckner Hartree-Fock, hole-line expansion … (*in 1960s, 70s*)

Relativistic BHF for finite nuclei
Shen, Hu, HZL, Meng, Ring, Zhang,
Chin. Phys. Lett. **33**, 102103 (2016)
Shen, HZL, Meng, Ring, Zhang,
PRC **96**, 014316 (2017)



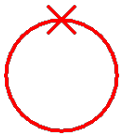
- **Functional Renormalization Group (FRG)** --- Wetterich, *PLB* **301**, 90 (1993)

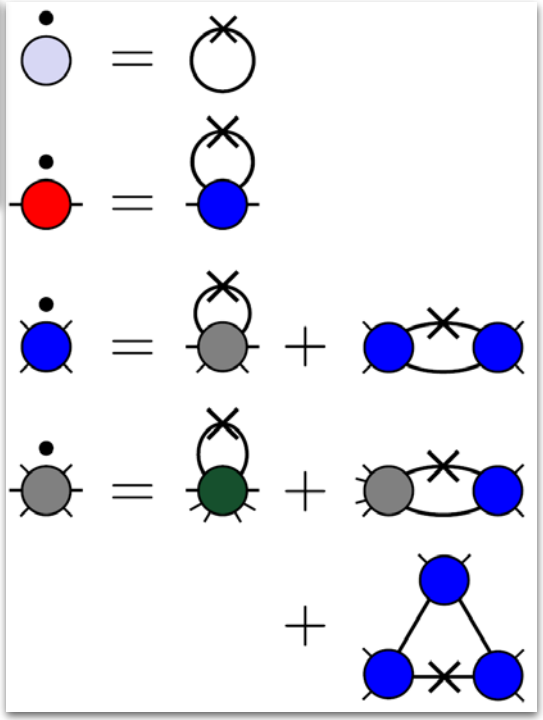
Exact evolution equation for the effective potential

Christof Wetterich
Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, W-6900 Heidelberg, FRG

Flow equation

$$\frac{\partial}{\partial k}\Gamma_k[\phi] = \frac{1}{2}\mathrm{Tr}\left\{\left[\Gamma_k^{(2)}[\phi] + R_k\right]^{-1}\frac{\partial}{\partial k}R_k\right\} = \frac{1}{2}$$





Cited 1700+ times *(google scholar, June 2019)*
in QCD, hadron, nuclear, cold atom, condensed matter, quantum chemistry ……

Non-perturbative nature of interaction

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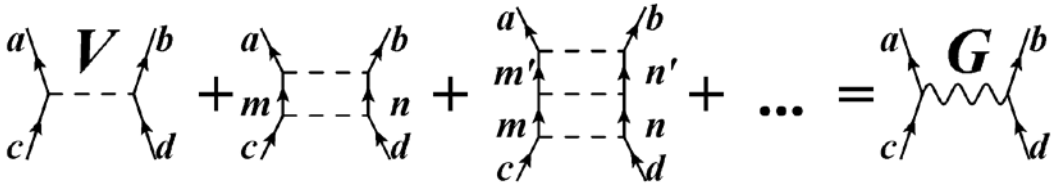
Chin. Phys. Lett. **33**, 102103 (2016)
Shen, HZL, Meng, Ring, Zhang,
PRC **96**, 014316 (2017)

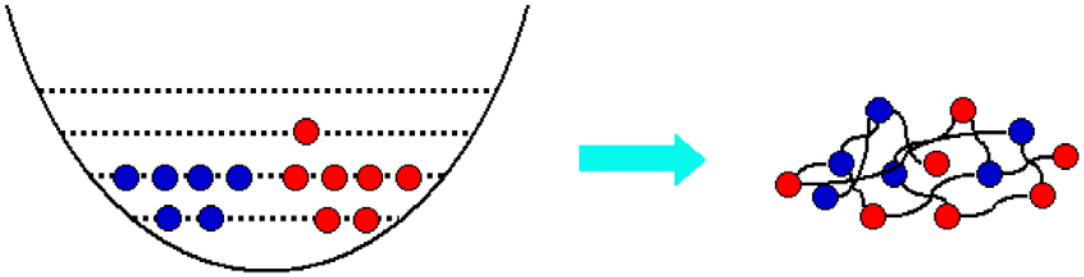


- **Functional Renormalization Group (FRG)** --- Wetterich, *PLB* **301**, 90 (1993)

- **FRG + DFT ---** Schwenk & Polonyi, arXiv:0403011 [nucl-th]

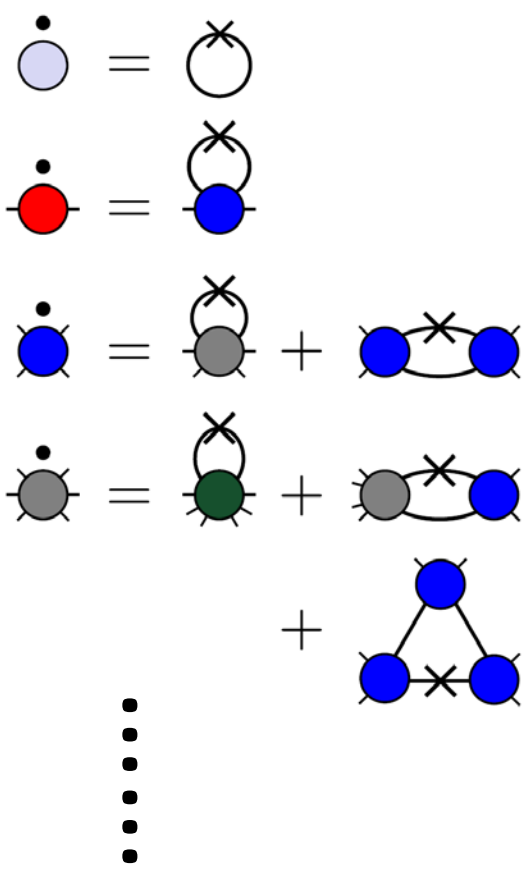
Flow equation

$$\partial_\lambda \Gamma_\lambda[\rho] = \mathrm{Tr}\left\{(\partial_\lambda U_\lambda)\cdot\rho + \frac{1}{2}\rho\cdot V\cdot\rho + \frac{1}{2}V\cdot\left[\Gamma_\lambda^{(2)}\right]^{-1}\right\}$$



Theoretical uncertainty

- **FRG Flow equation:** a set of coupled differential equations (infinite hierarchy)



To solve exactly?

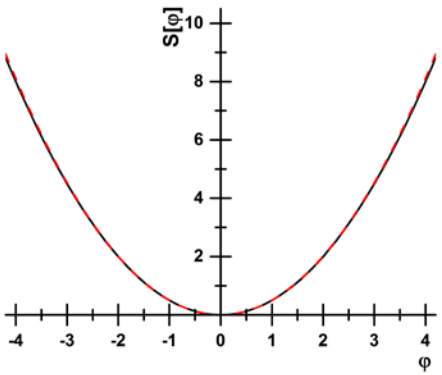
To estimate smartly?

- Proper power counting by $\Gamma^{(0)}$, $\Gamma^{(2)}$, $\Gamma^{(3)}$, $\Gamma^{(4)}$ …?
- Controllable theoretical uncertainty?

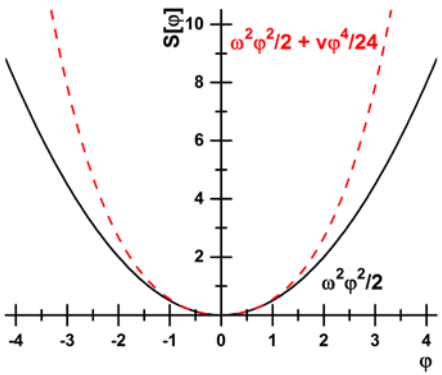
Contents

- Introduction
- Case study: φ^4-theory in zero dimension

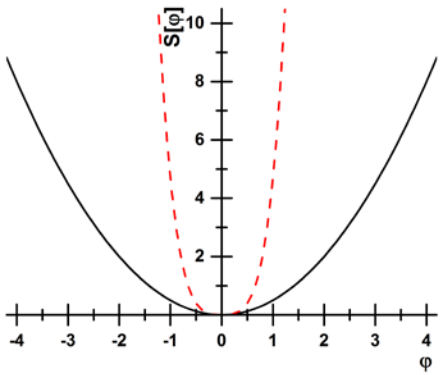
  cf. Kemler & Braun, *JPG* **40**, 085105 (2013)
- Results and Discussion
- Summary



perturbative



non-perturbative



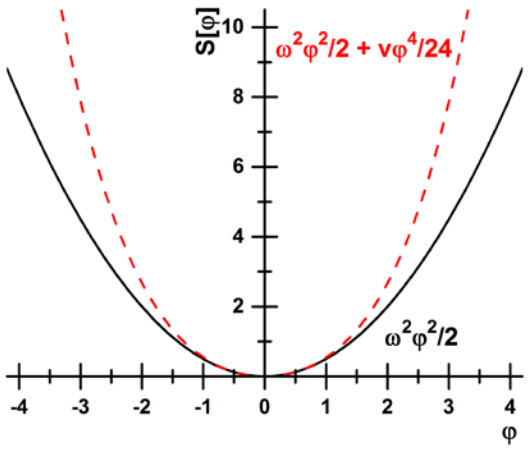
highly non-perturbative

φ^4-theory in zero dimension

Model setup

- **Classical action** (0D in space-time, bosonic d.o.f.)

$$S[\varphi] = \frac{1}{2}\omega^2\varphi^2 + \frac{1}{24}v\varphi^4$$



- **Partition function** (2PPI scheme)

$$Z[J] = \int_{-\infty}^{\infty} \mathrm{d}\varphi \, \exp\{-S[\varphi] + J\varphi^2\}$$

Exact solution

- Ground-state energy ($v_0 = v/\omega^4$)

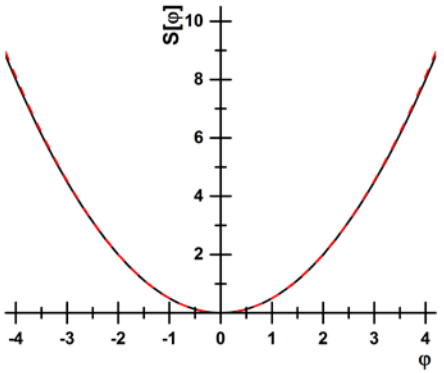
$$E_{\mathrm{gs}} = Z[0]/Z_0 = \int_{-\infty}^{\infty} \mathrm{d}\varphi \, \exp\{-S[\varphi]\}/Z_0 = \sqrt{\frac{3}{2\pi v_0}}\, K_{\frac{1}{4}}\left(\frac{3}{4v_0}\right) e^{\frac{3}{4v_0}}$$

- Ground-state density

$$\rho_{\mathrm{gs}} = \langle\varphi^2\rangle = \frac{1}{Z}\frac{\delta Z[J]}{\delta J}\bigg|_{J=0}$$
$$= \frac{1}{\omega^2}\left[\frac{3}{2}K_{\frac{5}{4}}\left(\frac{3}{4v_0}\right) + \frac{3}{2}K_{-\frac{3}{4}}\left(\frac{3}{4v_0}\right) - (v_0+3)K_{\frac{1}{4}}\left(\frac{3}{4v_0}\right)\right] \Big/ \left[v_0 K_{\frac{1}{4}}\left(\frac{3}{4v_0}\right)\right]$$

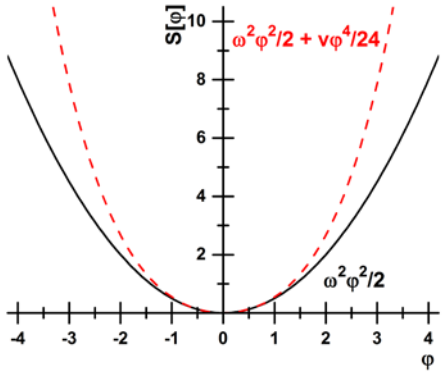
Typical cases

$v/\omega^4 = 0.01$



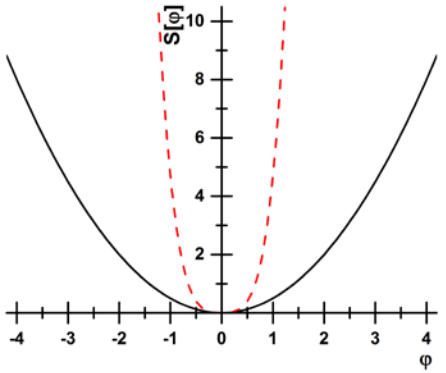
perturbative

$v/\omega^4 = 1$

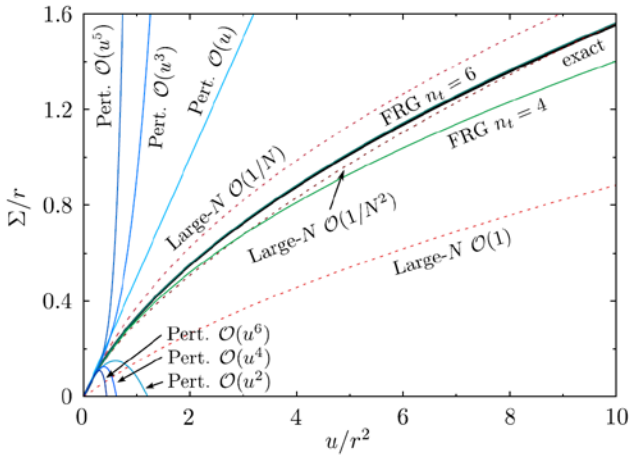


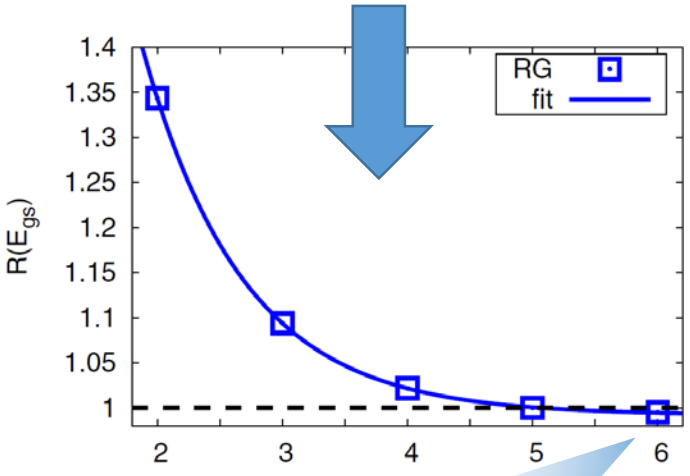
non-perturbative

$v/\omega^4 = 100$



highly non-perturbative





barely discussed

$$\rho_{\rm gs} = \omega^{-2}\left(1 - \frac{v_0}{2} + \frac{2v_0^2}{3} - \frac{11v_0^3}{8} + \frac{34v_0^4}{9} + \dots\right)$$

$$E_{\rm gs} = \frac{v_0}{8} - \frac{v_0^2}{12} + \frac{11v_0^3}{96} - \frac{17v_0^4}{72} + \dots$$

2% error in 6th-order cal.

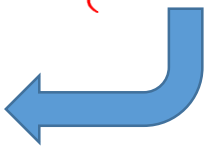
Keitel & Bartosch, *JPA* **45**, 105401 (2012)
Kemler & Braun, *JPG* **40**, 085105 (2013)

FRG for 0D φ^4-theory

- **FRG + DFT Flow equation**

$$\partial_\lambda \Gamma_\lambda[\rho] = \mathrm{Tr}\left\{(\partial_\lambda U_\lambda)\cdot\rho + \frac{1}{2}\rho\cdot V\cdot\rho + \frac{1}{2}V\cdot\left[\Gamma^{(2)}_\lambda\right]^{-1}\right\}$$

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24} v\left[\rho^2 + \left(\Gamma^{(2)}_\lambda[\rho]\right)^{-1}\right]$$



- **Conventional expansion** Kemler & Braun, *JPG* **40**, 085105 (2013)

$$\Gamma_\lambda[\rho] = \Gamma^{(0)}_\lambda[\bar\rho_\lambda] + \sum_{n=2}^{\infty}\frac{1}{n!}\Gamma^{(n)}_\lambda[\bar\rho_\lambda](\rho-\bar\rho_\lambda)^n$$

- **Coupled differential equations**

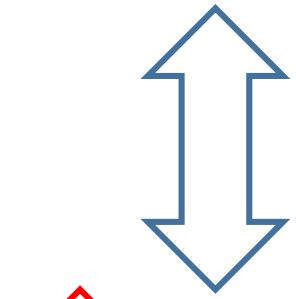
$$\partial_\lambda \Gamma^{(0)}_\lambda[\bar\rho_\lambda] = \frac{1}{24} v\left[\bar\rho^2_\lambda + G_\lambda[\bar\rho_\lambda]\right]$$

$$\partial_\lambda \bar\rho_\lambda = -\frac{1}{24} v\left[2\bar\rho_\lambda\, G_\lambda[\bar\rho_\lambda] - \Gamma^{(3)}_\lambda[\bar\rho_\lambda] G^3_\lambda[\bar\rho_\lambda]\right]$$

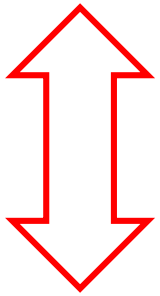
$$\partial_\lambda \Gamma^{(2)}_\lambda[\bar\rho_\lambda] = \frac{1}{24} v\left[2 + 3(\Gamma^{(3)}_\lambda)^2 G^3_\lambda - 2\rho\Gamma^{(3)}_\lambda G_\lambda\right]_{\bar\rho_\lambda}$$

$$\partial_\lambda \Gamma^{(3)}_\lambda[\bar\rho_\lambda] = -\frac{1}{4} v\left[(\Gamma^{(3)}_\lambda)^3 G^4_\lambda\right]_{\bar\rho_\lambda}$$

$\vdots$



To slove



Setting to zero

FRG for 0D φ^4-theory

- **FRG + DFT Flow equation**

$$\partial_\lambda \Gamma_\lambda[\rho] = \mathrm{Tr}\left\{(\partial_\lambda U_\lambda)\cdot\rho + \frac{1}{2}\rho\cdot V\cdot\rho + \frac{1}{2}V\cdot\left[\Gamma^{(2)}_\lambda\right]^{-1}\right\}$$

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24} v\left[\rho^2 + \left(\Gamma^{(2)}_\lambda[\rho]\right)^{-1}\right]$$

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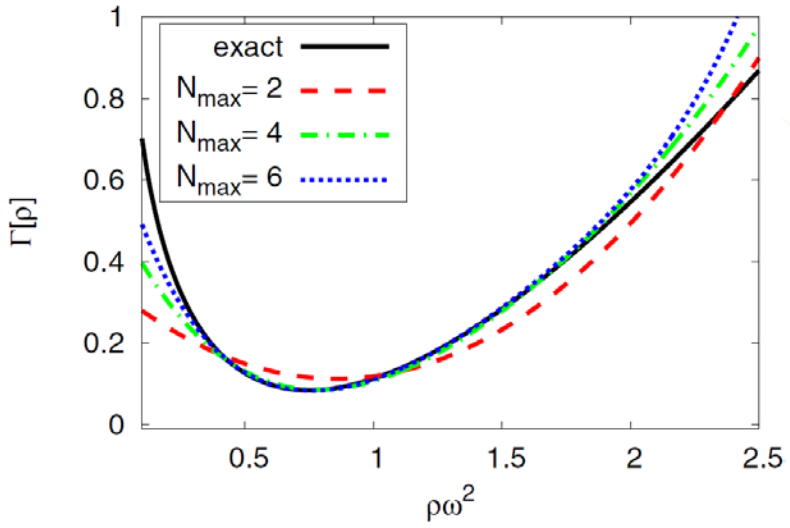
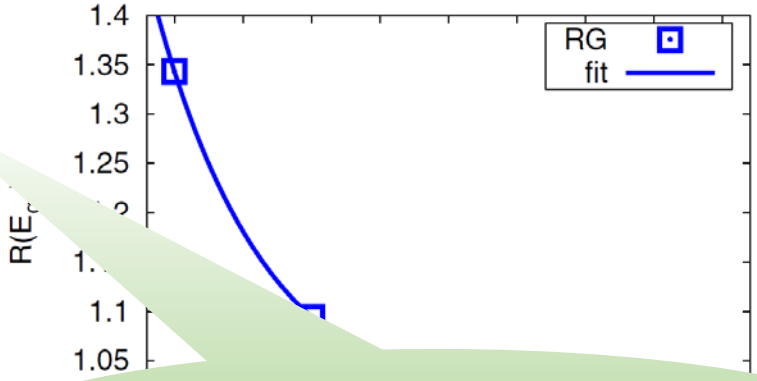
$$\Gamma_\lambda[\rho] = \Gamma^{(0)}_\lambda[\bar\rho_\lambda] + \sum_{n=2}^{\infty}\frac{1}{n!}\Gamma^{(n)}_\lambda[\bar\rho_\lambda](\rho-\bar\rho_\lambda)^n$$





- **Kohn-Sham scheme?**
- **uncertainties?**

- Up to 6th-order calculation, results are not satisfactory.

Our ideas

- **FRG + DFT Flow equation**

$$\partial_\lambda \Gamma_\lambda[\rho] = \mathrm{Tr}\left\{(\partial_\lambda U_\lambda)\cdot\rho + \frac{1}{2}\rho\cdot V\cdot\rho + \frac{1}{2}V\cdot\left[\Gamma_\lambda^{(2)}\right]^{-1}\right\}$$

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24} v\left[\rho^2 + \left(\Gamma_\lambda^{(2)}[\rho]\right)^{-1}\right]$$

- **Optimized expansion (KS-FRG)**

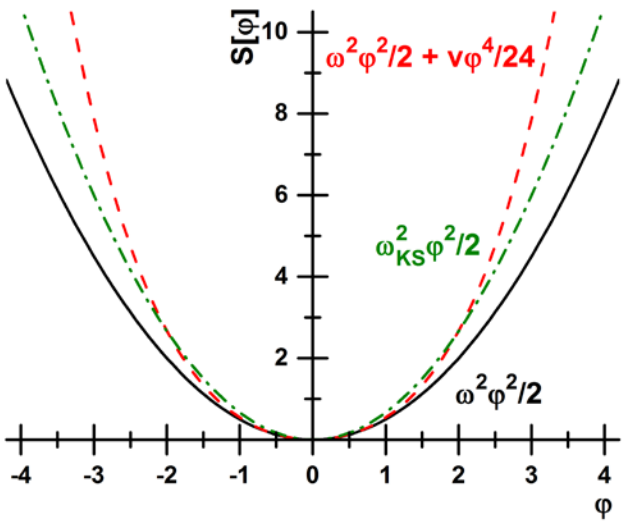
$$\Gamma_\lambda[\rho] = \Gamma_{\mathrm{KS},\lambda}[\rho] + \gamma_\lambda[\rho]$$

  - **Non-interacting part**

$$\Gamma_{\mathrm{KS},\lambda}[\rho] = -\frac{1}{2}\ln(\omega^2\rho) - \frac{1}{2} + \frac{\rho}{2\bar{\rho}_\lambda}$$

  - **Correlation part**

$$\gamma_\lambda[\rho] = \gamma_\lambda^{(0)}[\bar{\rho}_\lambda] + \sum_{n=2}^{\infty}\frac{1}{n!}\gamma_\lambda^{(n)}[\bar{\rho}_\lambda](\rho-\bar{\rho}_\lambda)^n$$



HZL, Niu, Hatsuda, *Phys. Lett. B* 779, 436 (2018)

Ideas of Kohn-Sham

- To introduce an artificial **non-interacting** system which provides **the same** ground-state density ρ_{gs} with a **Kohn-Sham** (mean-field) **potential**
- **Difference** between interacting and non-interacting systems is absorbed in the correlation (***beyond-mean-field***) part of EDF, $E_x[\rho]$.

KS - FRG

- **Coupled differential equations ← Optimized FRG + DFT**

$$\partial_\lambda \bar{\rho}_\lambda = -\frac{1}{24} v \left[2\rho G_\lambda + (\frac{1}{\rho^3} - \gamma_\lambda^{(3)}) G_\lambda^3 \right]_{\bar{\rho}_\lambda}$$

$$\partial_\lambda \gamma_\lambda^{(0)}[\bar{\rho}_\lambda] = \frac{1}{24} v \left[\rho^2 - \frac{1}{2\rho} (\frac{1}{\rho^3} - \gamma_\lambda^{(3)}) G_\lambda^3 \right]_{\bar{\rho}_\lambda}$$

$$\partial_\lambda \gamma_\lambda^{(2)}[\bar{\rho}_\lambda] = \frac{1}{24} v \left[2 - 2\rho\gamma_\lambda^{(3)} G_\lambda - (\frac{3}{\rho^4} + \gamma_\lambda^{(4)}) G_\lambda^2 + (\frac{1}{\rho^3} - \gamma_\lambda^{(3)})(\frac{2}{\rho^3} - 3\gamma_\lambda^{(3)}) G_\lambda^3 \right]_{\bar{\rho}_\lambda}$$

$$\partial_\lambda \gamma_\lambda^{(3)}[\bar{\rho}_\lambda] = \frac{1}{24} v \left[-2\rho\gamma_\lambda^{(4)} G_\lambda + \frac{12}{\rho^5} G_\lambda^2 - (\frac{1}{\rho^3} - \gamma_\lambda^{(3)})(\frac{18}{\rho^4} + 7\gamma_\lambda^{(4)}) G_\lambda^3 + 6(\frac{1}{\rho^3} - \gamma_\lambda^{(3)})^3 G_\lambda^4 \right]_{\bar{\rho}_\lambda}$$

$$\partial_\lambda \gamma_\lambda^{(4)}[\bar{\rho}_\lambda] = \frac{1}{24} v \left[-\frac{60}{\rho^6} G_\lambda^2 + \frac{96}{\rho^5} (\frac{1}{\rho^3} - \gamma_\lambda^{(3)}) G_\lambda^3 + 6(\frac{3}{\rho^4} + \gamma_\lambda^{(4)})^2 G_\lambda^3 \right.$$
$$\left. -36(\frac{1}{\rho^3} - \gamma_\lambda^{(3)})^2 (\frac{3}{\rho^4} + \gamma_\lambda^{(4)}) G_\lambda^4 + 24(\frac{1}{\rho^3} - \gamma_\lambda^{(3)})^4 G_\lambda^5 \right]_{\bar{\rho}_\lambda}$$

⋮

To solve

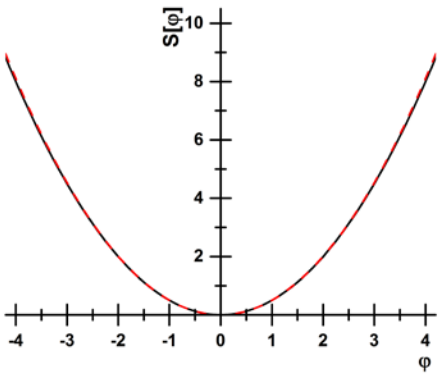
Estimating upper/lower bounds

Keeping as KS counterparts

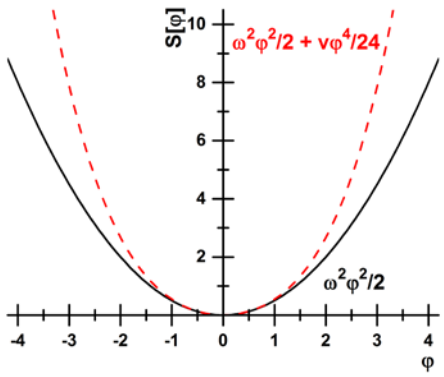
Contents

- Introduction
- Case study: φ^4-theory in zero dimension

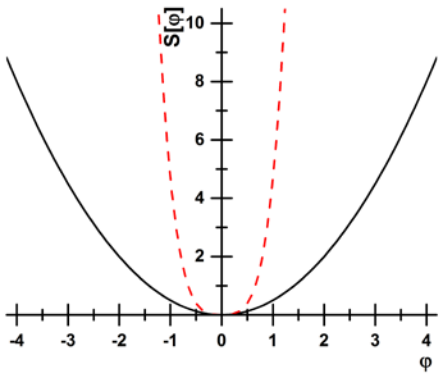
  cf. Kemler & Braun, JPG 40, 085105 (2013)
- Results and Discussion
- Summary



perturbative

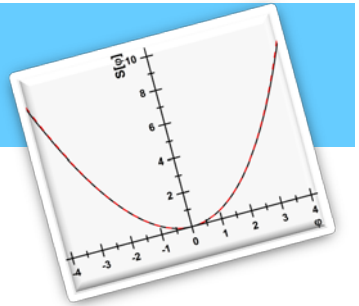


non-perturbative

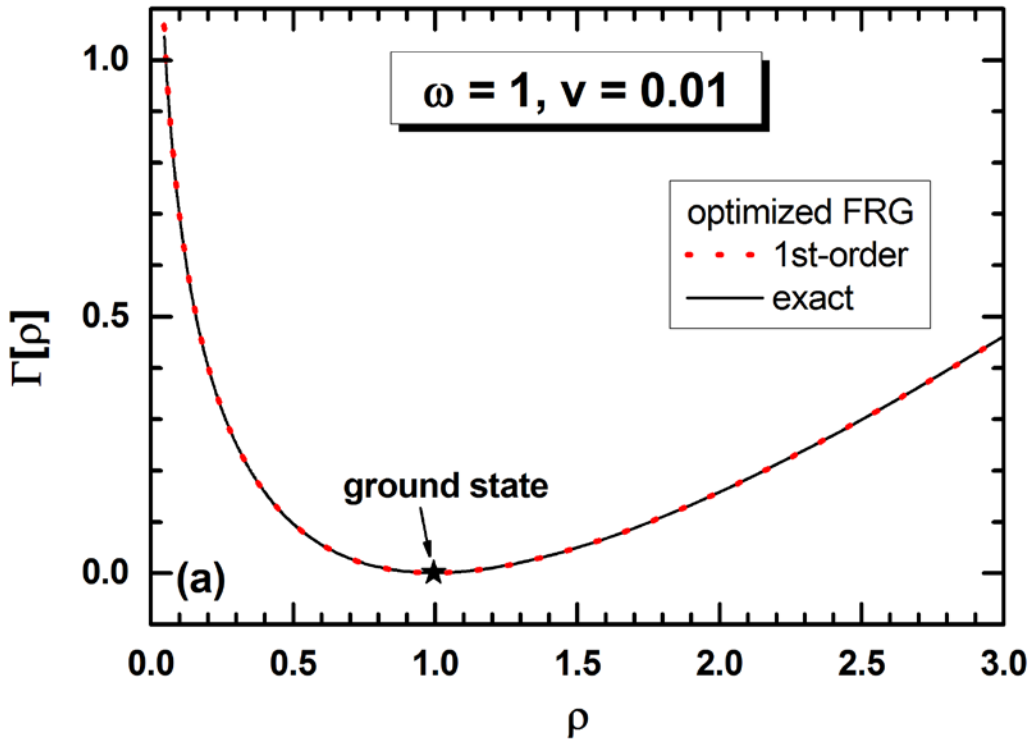


highly non-perturbative

Typical cases (I)



- **Perturbative case $v_0 = v/\omega^4 = 0.01$**

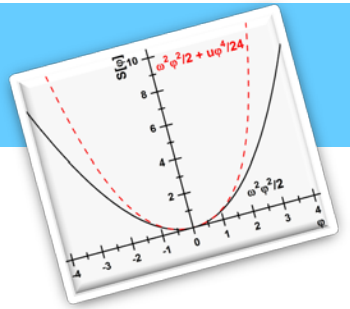


- Effective action *vs* density, $F_{HK}[\rho]$.

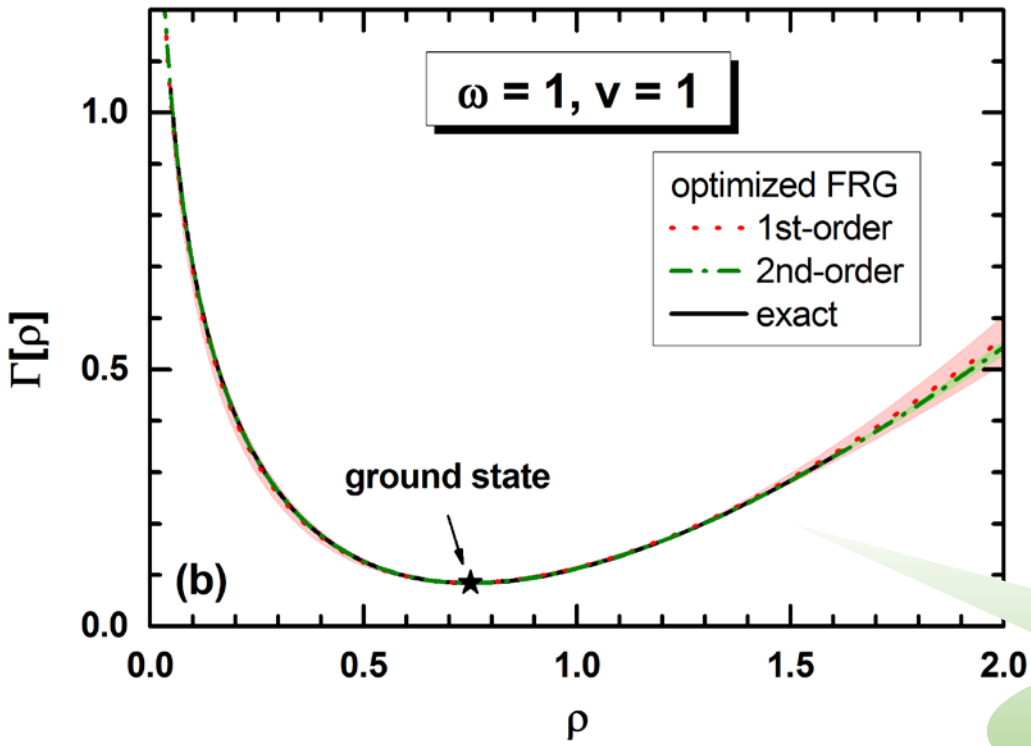
HZL, Niu, Hatsuda, *Phys. Lett. B* 779, 436 (2018)

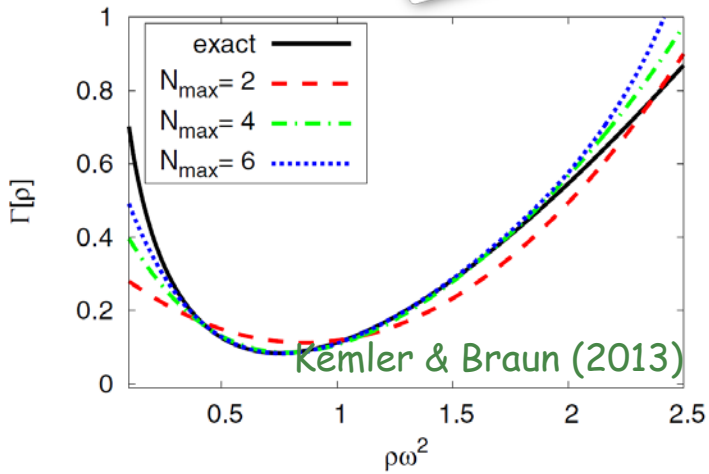
- **1st-order optimized FRG** result is on top of the **exact solution** in a very large density region.
- **Theoretical uncertainty** is invisible in the figure.

Typical cases (II)



- **Non-perturbative case $v_0 = v/\omega^4 = 1$**





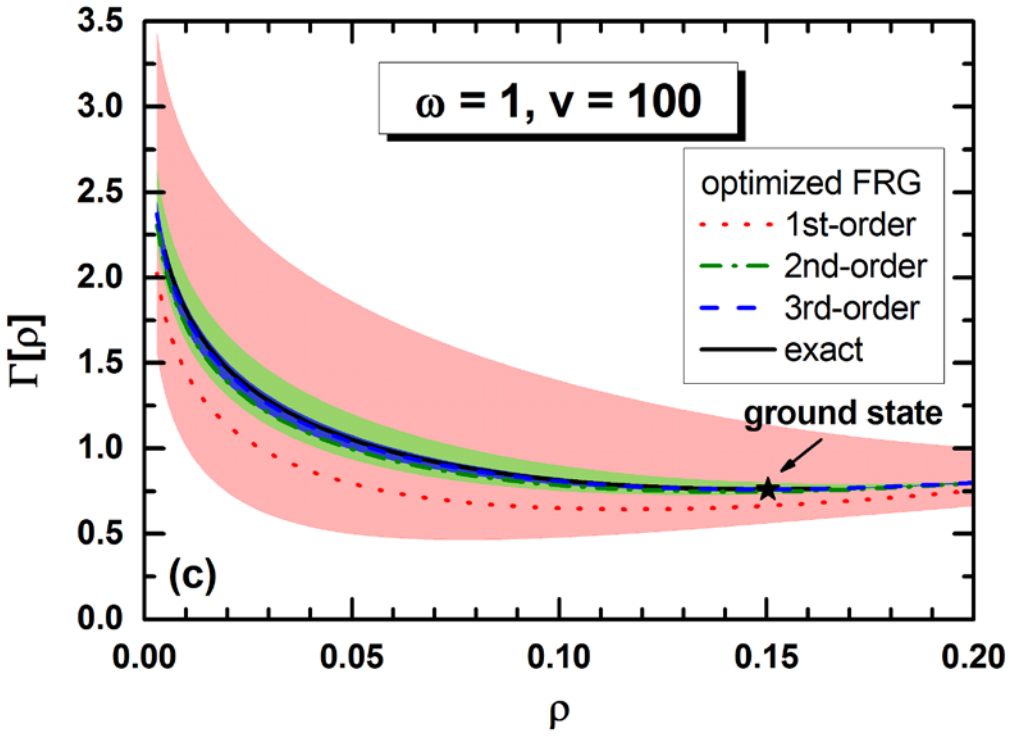
- Effective action *vs* density, $F_{HK}[\rho]$.

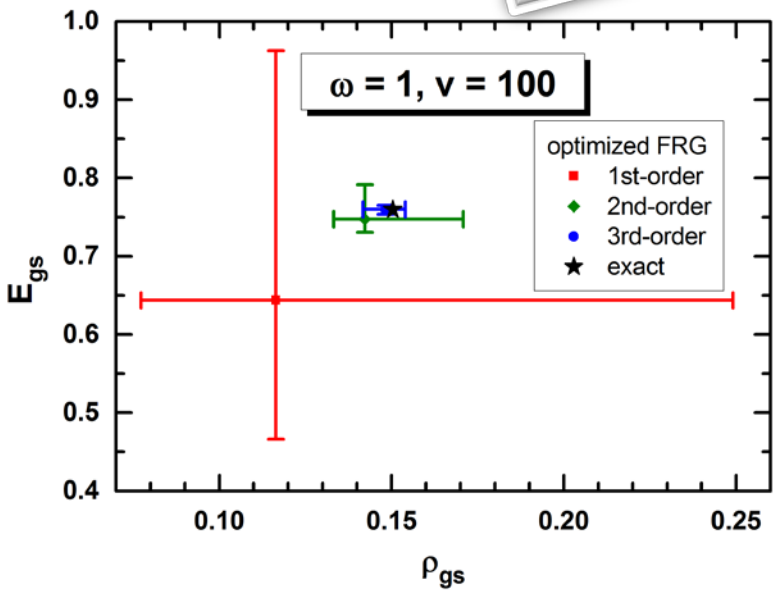
KS optimized FRG

- **1st-order result** reproduces the **exact solution** in a wide density region, with corresponding **uncertainty**.
- **2nd-order result** does improve.

Typical cases (III)

- **Highly non-perturbative case $v_0 = v/\omega^4 = 100$**





◆ Ground-state density and energy.

- **1st-order result** is still able to describe the **exact solution** with large **uncertainty**.
- **2nd-order and 3rd-order results** improve step by step

  — **accuracy** of ρ_{gs} increases by factor **4**, E_{gs} by factor **10** at each order.

Ground-state properties

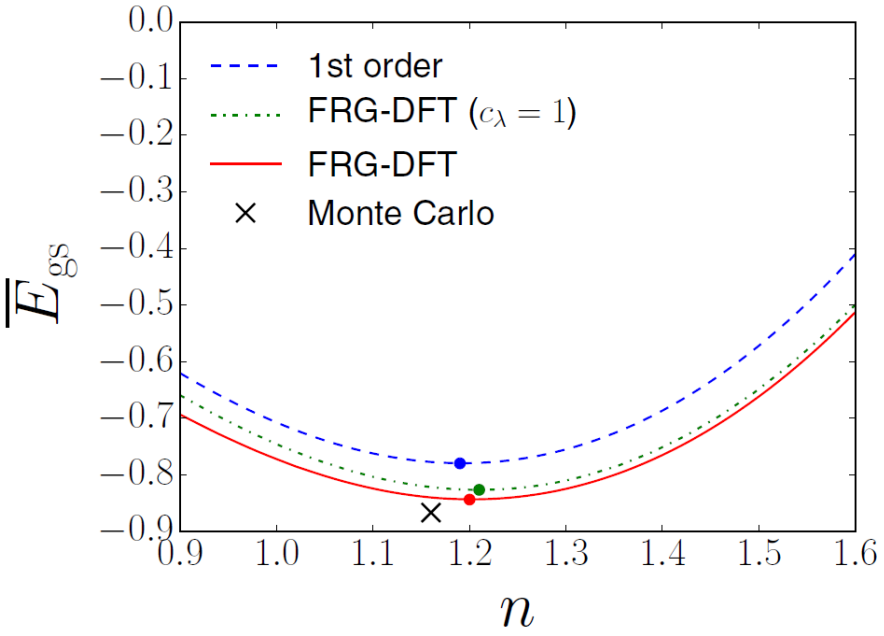
- Ground-state densities and energies: φ^4-theory in 0D

	$v = 0.01$		$v = 1$		$v = 100$	
	$\rho_{\rm gs}$	$E_{\rm gs}$	$\rho_{\rm gs}$	$E_{\rm gs}$	$\rho_{\rm gs}$	$E_{\rm gs}$
1st-order	0.99506529^{+27}_{-77}	$0.00124178 5^{+55}_{-19}$	0.745^{+18}_{-23}	0.0850^{+11}_{-10}	0.12^{+13}_{-4}	0.64^{+32}_{-18}
2nd-order	0.99506530^{+8}_{-20}	$0.00124177880^{+31}_{-81}$	0.7508^{+14}_{-11}	0.08456^{+36}_{-45}	0.142^{+29}_{-9}	0.747^{+44}_{-17}
3rd-order	0.9950653285^{+21}_{-8}	$0.00124177894 4^{+16}_{-44}$	0.75052^{+15}_{-15}	0.084529^{+67}_{-68}	0.1482^{+58}_{-65}	0.7597^{+52}_{-62}
exact	0.995065328 2	0.00124177895 1	0.75051	0.084557	0.1504	0.7597

$8^{\rm th}$ digit **0.08%** **0.8%**

Progress in 1D & 2D systems

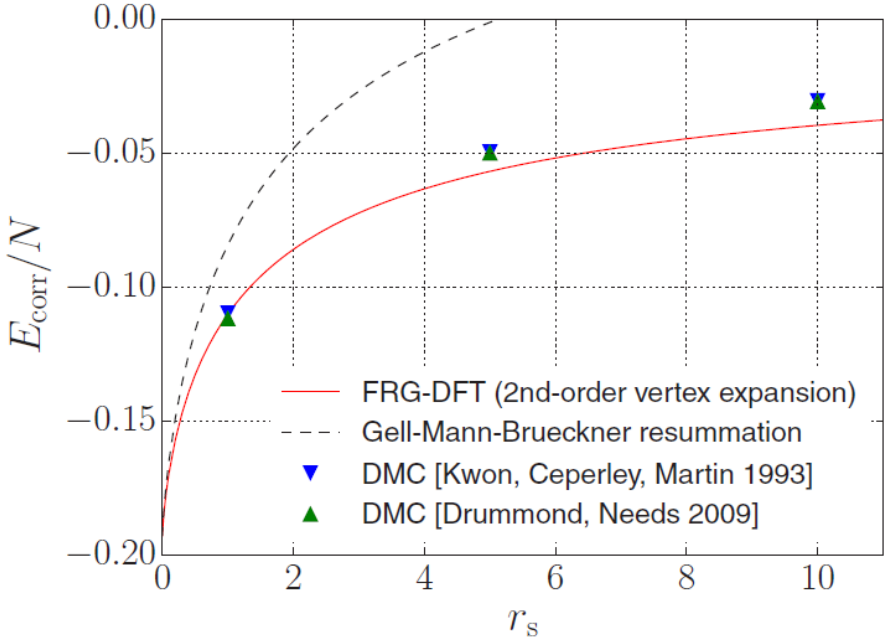
- EoS of 1D nuclear matter



Yokota, Yoshida, Kunihiro,
Phys. Rev. C **99**, 024302 (2019)
PTEP **2019**, 011D01 (2019)

cf.
Kemler, Pospiech, Braun, *JPG* **44**, 015101 (2017)
Alexandrou, Myczkowski, Negele, *PRC* **39**, 1076 (1989)

- Correlation energy of 2D electron gas

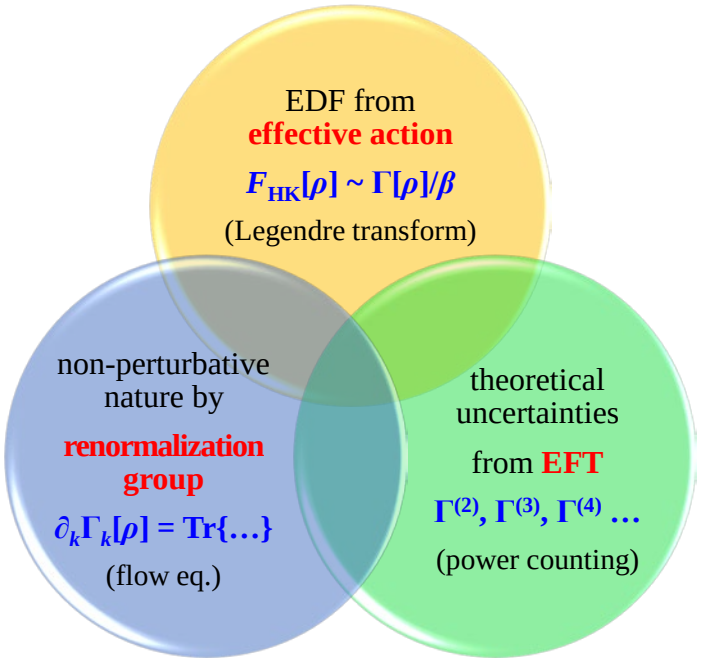


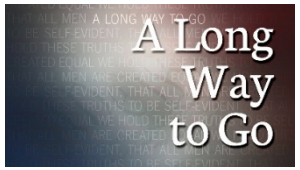
Yokota & Naito, *Phys. Rev. B* **99**, 115106 (2019)

Summary

DFT ← ideas of QFT (effective action + RG + EFT)

- ✓ EDF $F_{HK}[\rho]$ is derived from effective action $\Gamma[\rho]$ in **2PPI** scheme with **Legendre transform**.
- ✓ Non-perturbative nature of interaction is handled by **FRG** with **flow equation**.
- ✓ Beyond-mean-field effects $\gamma^{(n)}$ in $F_{HK}[\rho]$ are taken into account **order-by-order** with (proper) **theoretical uncertainties**.





from ***φ^4-theory in 0D***
to ***3+1D finite nuclei …***

Further reading

A shortest cut for understanding DFT

① W. Kohn, *Nobel Lecture: Electronic structure of matter—wave functions and density functionals*, *Rev. Mod. Phys.* **71**, 1253-1266 (1999).

② W. Kutzelnigg, *Density functional theory in terms of a Legendre transformation for beginners*, *J. Mol. Struct.* **768**, 163-173 (2006).

③ H. Eschrig, *The Fundamentals of Density Functional Theory (revised and extended version)* (EAG.LE, Leipzig 2003).

Recent reviews

- T. Nakatsukasa, K. Matsuyanagi, M. Matsuo, and K. Yabana, *Time-dependent density-functional description of nuclear dynamics*, *Rev. Mod. Phys.* **88**, 045004 (2016).
- R.O. Jones, *Density functional theory: Its origins, rise to prominence, and future*, *Rev. Mod. Phys.* **87**, 897-923 (2015).
- E.S. Kryachko and E.V. Ludena, *Density functional theory: Foundations reviewed*, *Phys. Rep.* **544**, 123-239 (2014).

Toward future developments

- J.E. Drut, R.J. Furnstahl, and L. Platter, *Toward ab initio density functional theory for nuclei*, *Prog. Part. Nucl. Phys.* **64**, 120-168 (2010).

Homework

"The Kohn-Sham reference system, that has originally been introduced as a tool without any physical meaning, just in order to circumvent the need to express the kinetic energy as a functional of the density, has turned out to carry more physics than originally believed."

Kutzelnigg, *J. Mol. Struct.* **768**, 163 (2006)

"What is the physics?"

Thank you!