*Workshop of Recent Developments in QCD and QFT*
*November 9-12, 2017, NTU, Taipei*

# Density Functional Theory with uncertainty quantification from Functional Renormalization Group in Kohn-Sham scheme

**Haozhao LIANG**（梁豪兆）

*RIKEN Nishina Center, Japan*
*Graduate School of Science, the University of Tokyo, Japan*

*November 11, 2017*

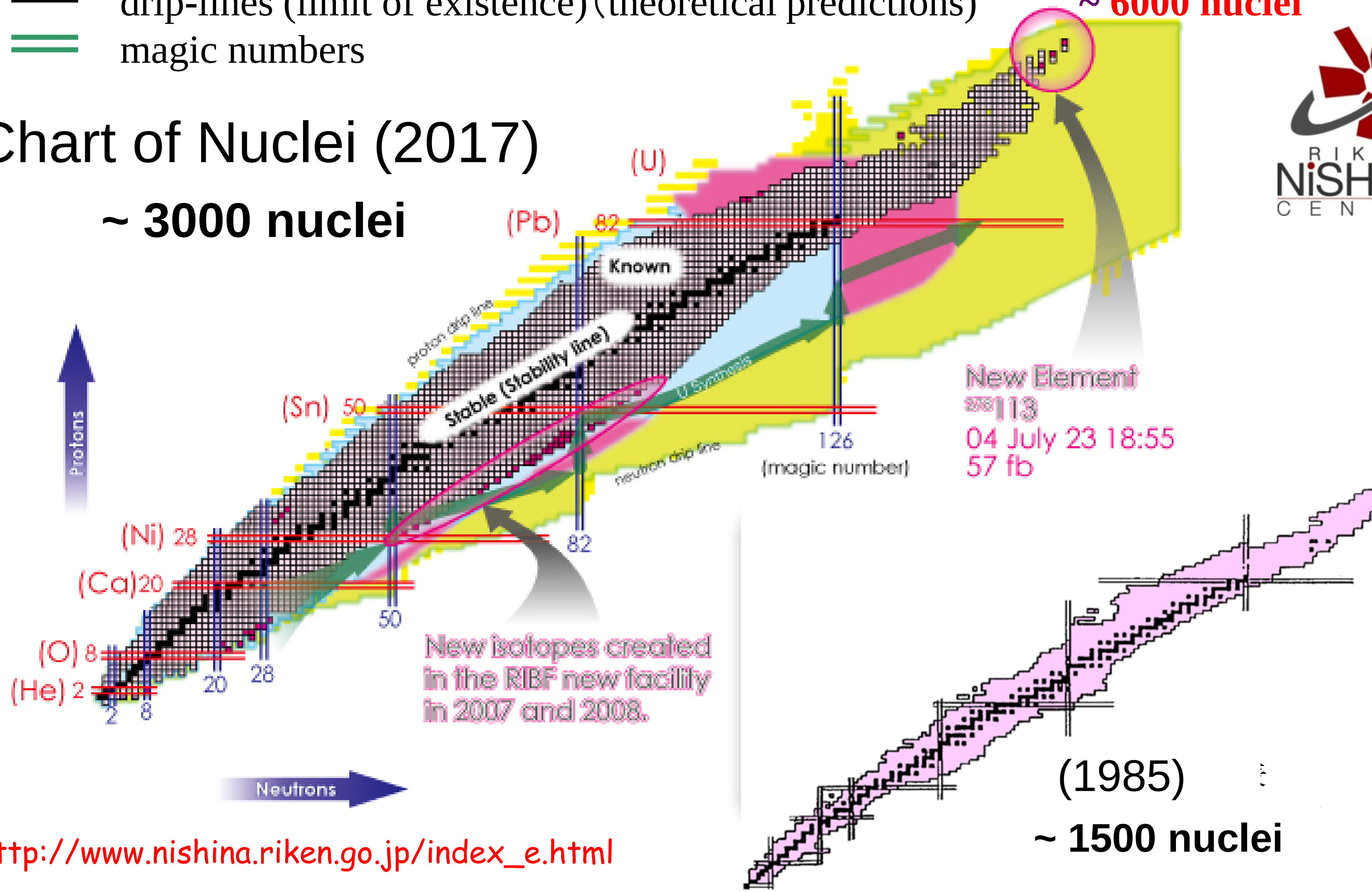
In collaboration with
**Tetsuo Hatsuda** (*RIKEN, Japan*) and **Yifei Niu** (*ELI-NP, Romania*)

# 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 (2017)

**~ 3000 nuclei**

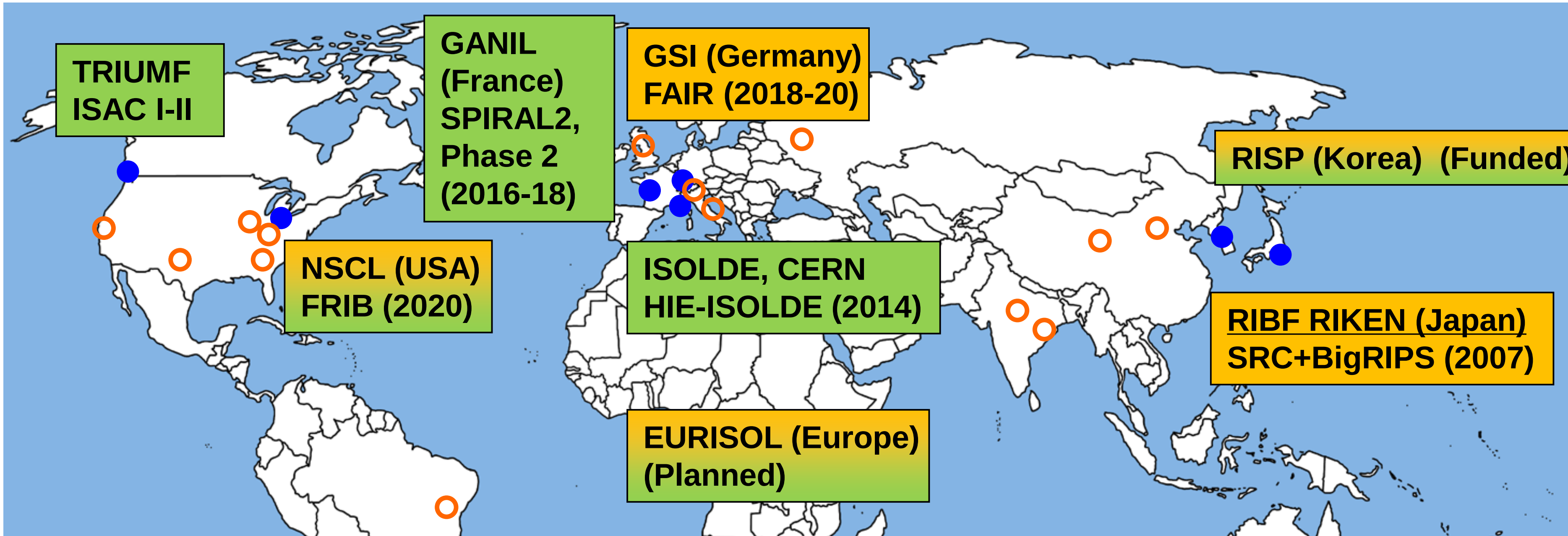



(1985)

**~ 1500 nuclei**

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

# Radioactive isotope beam facilities





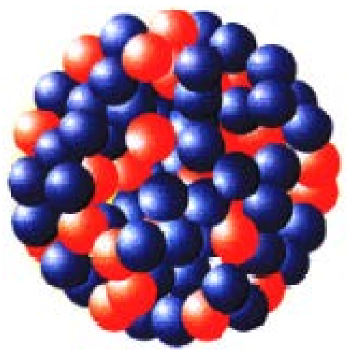
**Best in the world**
**~70 % speed of light !**

RIKEN NISHINA CENTER

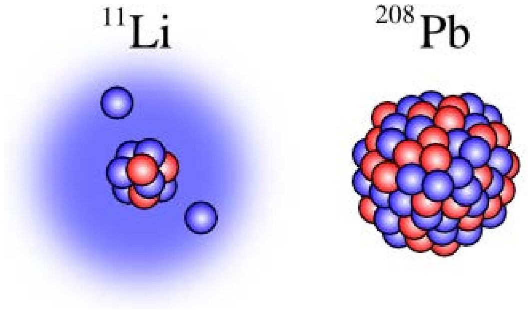
# Atomic nuclei

Atomic nucleus is a rich system in physics

- quantum system
- many-body system ($A$ ~ 100, spin & isospin d.o.f.)
- finite system (surface, skin, halo, …)
- open system (resonance, continuum, decay, …)



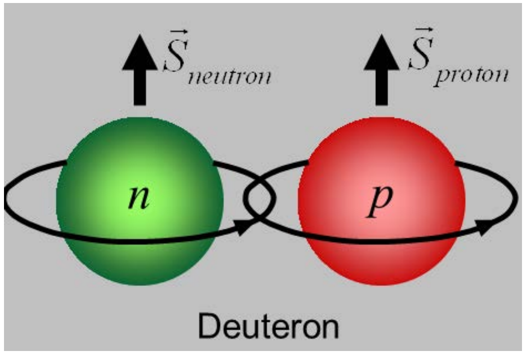
Neutron halos



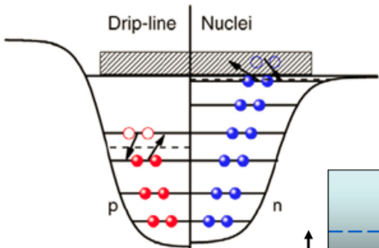

**$R \sim A^{1/3}$? Not always!**
**$^{11}$Li: a size as $^{208}$Pb**

Tanihata:1985

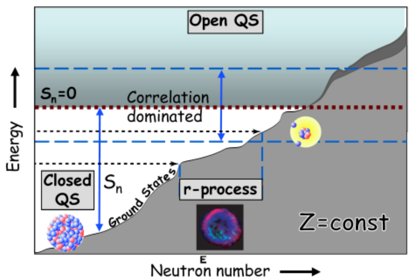
**Spin** and **Isospin** are essential degrees of freedom in nuclear physics.



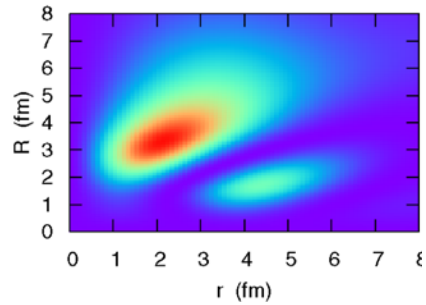
# Physics of exotic nuclei

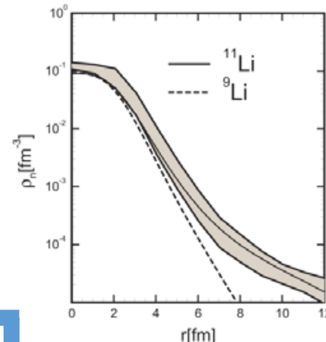



Weakly-bound




*Threshold*
*Continuum*
*Open Q.S.*

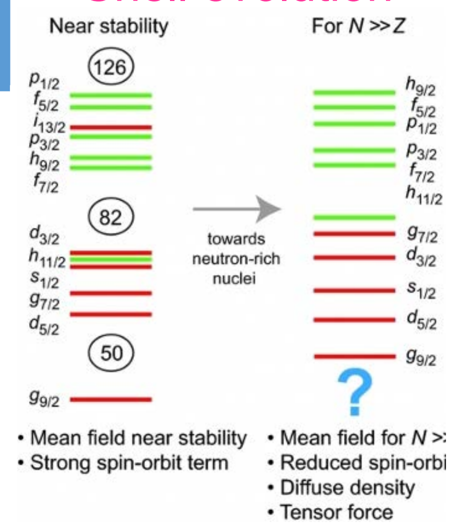


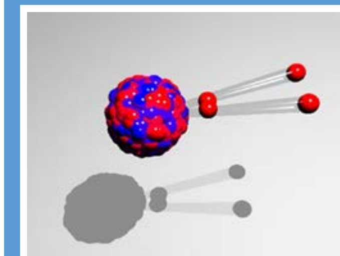

Halo

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

Shell evolution

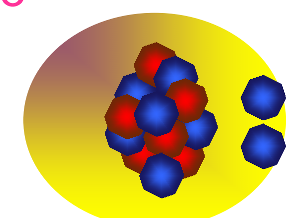


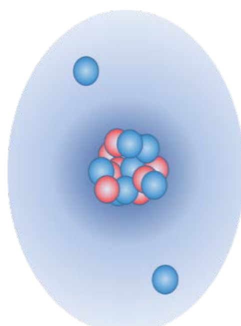

New radioact.



*1p emission*
*2p emission*
*2n emission*

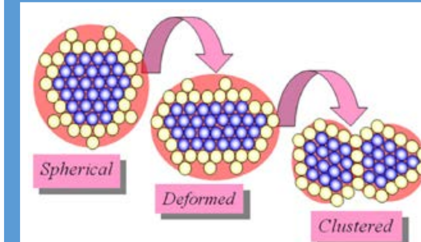
Halo

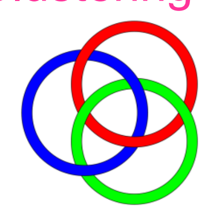




*Deformation*
*Shape decoupling*

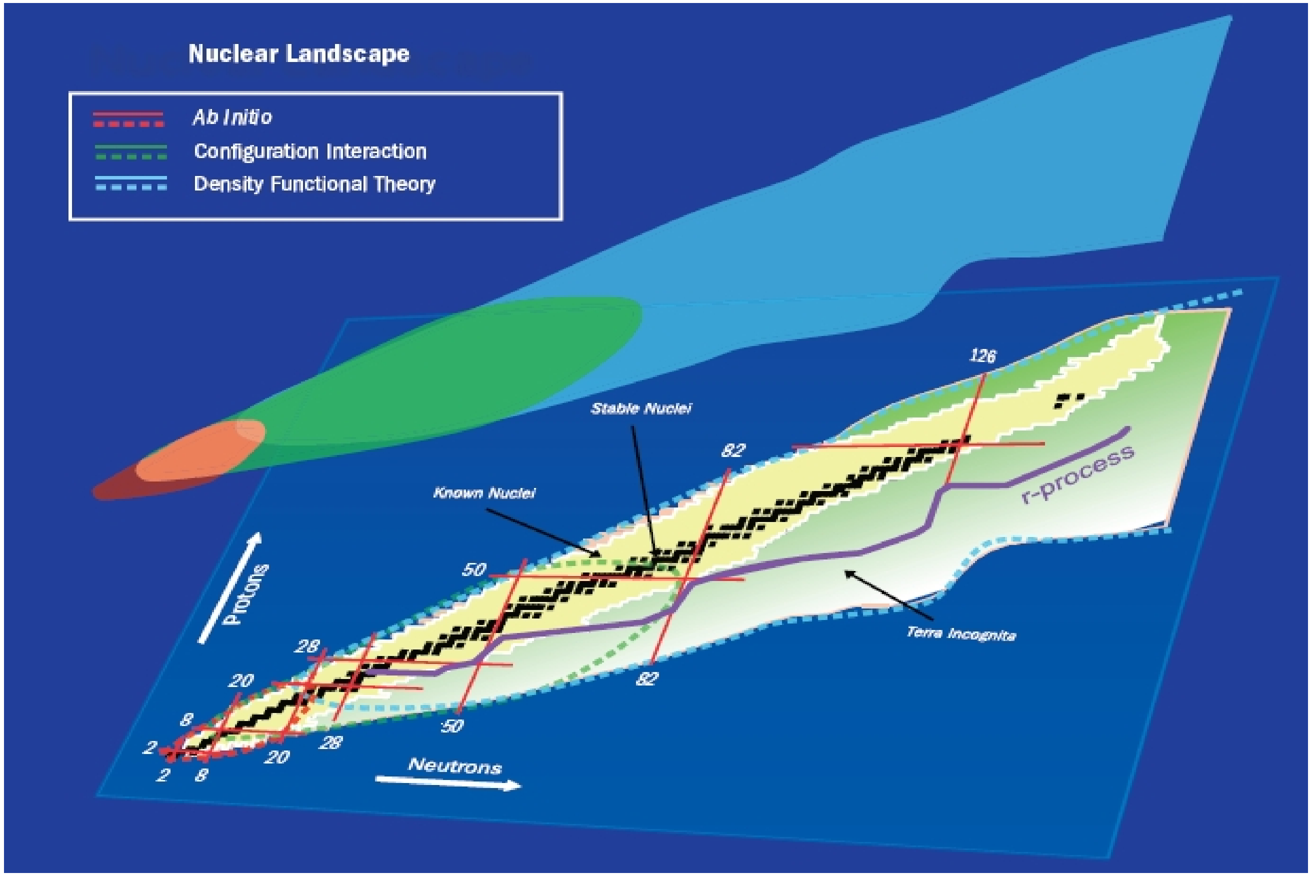
Clustering



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

# State-of-the-art nuclear methodologies




http://www.unedf.org/

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

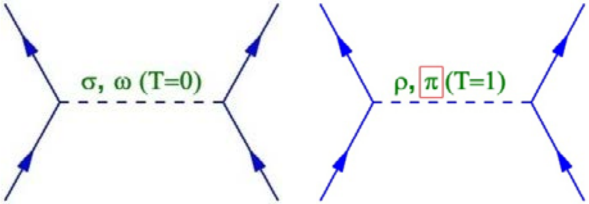
# Covariant density functional theory

## Covariant density functional theory (CDFT)

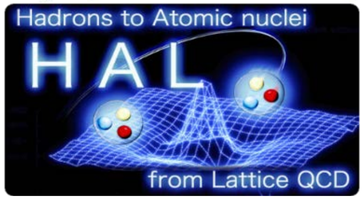
Nobel Prize 1949
Nobel Prize 1998

- Fundamental: **Kohn-Sham** Density Functional Theory
- Scheme: **Yukawa** meson-exchange nuclear interactions

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




**Comparing to traditional non-relativistic DFT**




Aoki *et al.*, *Prog. Theor. Exp. Phys.* **2012**, 01A105 (2012)

- Effective Lagrangian
  connections to underlying theories, QCD at low energy
- Dirac equation
  consistent treatment of **spin** d.o.f. & nuclear saturation properties (**3-body effect**)
- Lorentz covariant symmetry
  unification of time-even and **time-odd** components

# Dirac and RPA equations

- **Energy functional** of the system

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

- **Dirac equations** for the ground-state properties

$$\int d\boldsymbol{r}' h(\boldsymbol{r}, \boldsymbol{r}') \psi(\boldsymbol{r}') = \varepsilon \psi(\boldsymbol{r}), \quad \text{with} \quad \begin{aligned} h^{\rm kin}(\boldsymbol{r}, \boldsymbol{r}') &= [\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta M]\, \delta(\boldsymbol{r} - \boldsymbol{r}'), \\ h^{\rm D}(\boldsymbol{r}, \boldsymbol{r}') &= [\Sigma_T(\boldsymbol{r})\gamma_5 + \Sigma_0(\boldsymbol{r}) + \beta \Sigma_S(\boldsymbol{r})]\, \delta(\boldsymbol{r} - \boldsymbol{r}'), \\ h^{\rm E}(\boldsymbol{r}, \boldsymbol{r}') &= \begin{pmatrix} Y_G(\boldsymbol{r}, \boldsymbol{r}') & Y_F(\boldsymbol{r}, \boldsymbol{r}') \\ X_G(\boldsymbol{r}, \boldsymbol{r}') & X_F(\boldsymbol{r}, \boldsymbol{r}') \end{pmatrix}. \end{aligned}$$

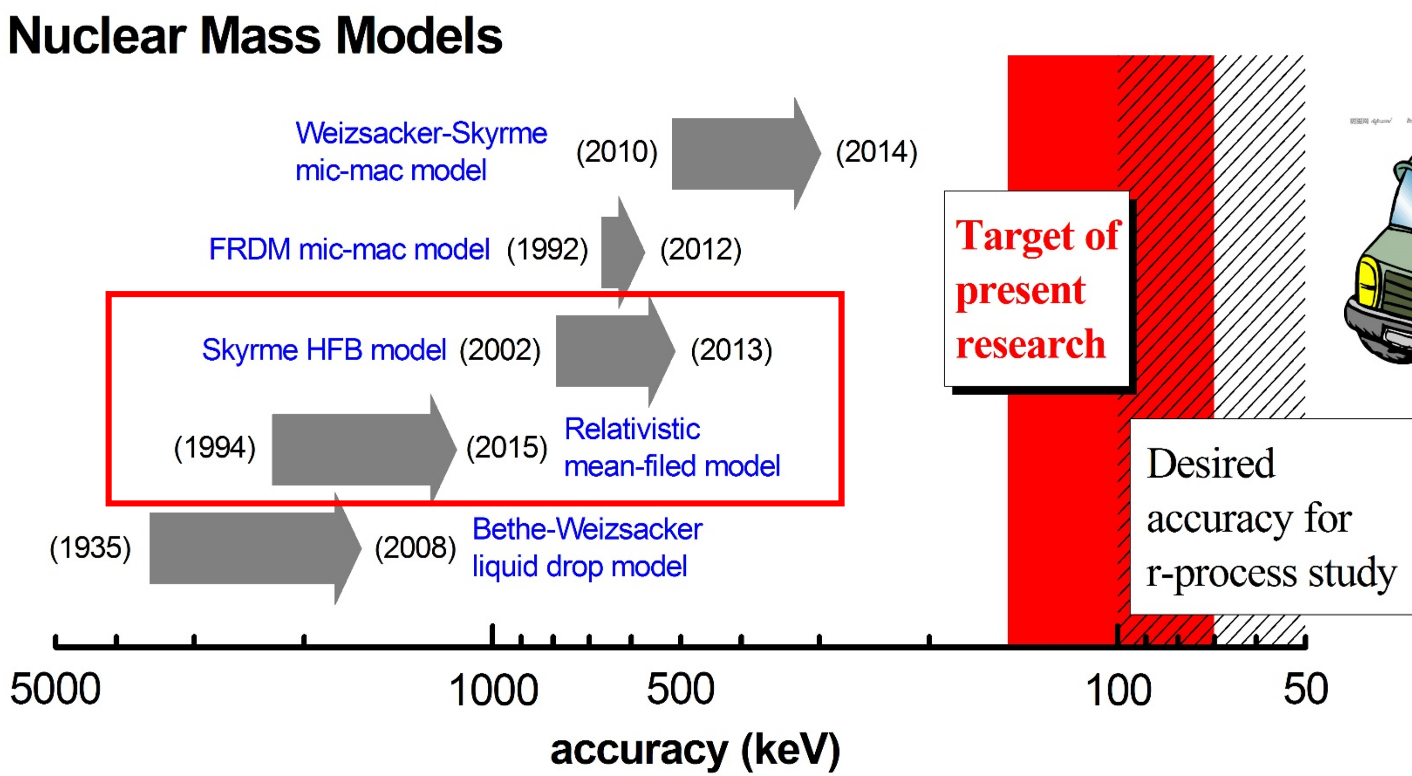
- **RPA equations** for the vibrational excitation properties

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega_\nu \begin{pmatrix} X \\ Y \end{pmatrix}$$

- $\delta E/\delta\rho$ → equation of motion for nucleons: Dirac (-Bogoliubov) equations
- $\delta^2 E/\delta\rho^2$ → linear response equation: (Q)RPA equations

Ring & Schuck, *The Nuclear Many-Body Problem* (Springer, New York, 1980)

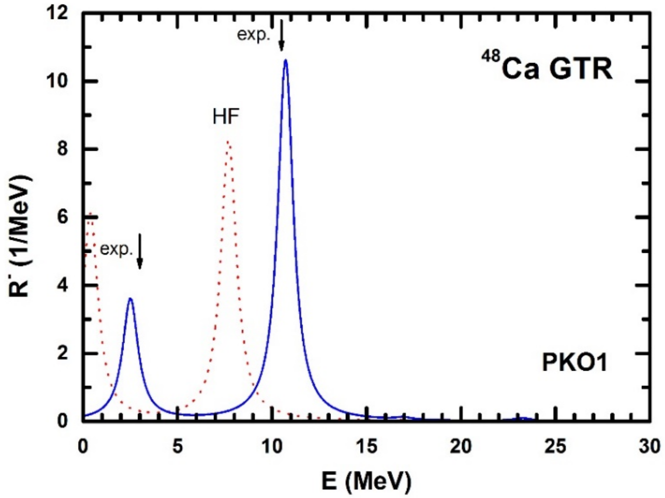
# Nuclear mass models

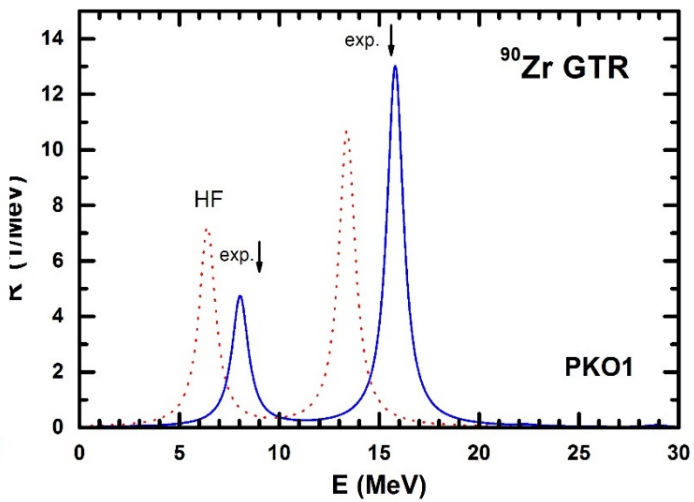



Accuracy for $^{208}$Pb: ~1/1600

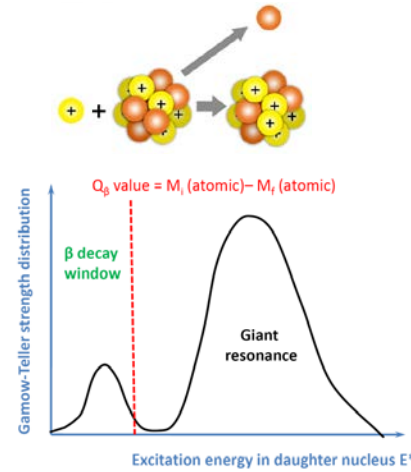
# Gamow-Teller resonances

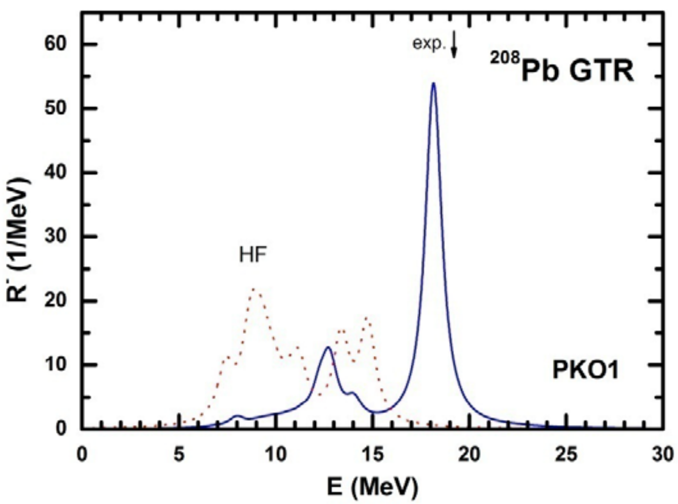
**CDFT+RPA** for Gamow-Teller resonances ($\Delta S = 1$, $\Delta L = 0$, $J^{\pi} = 1^{+}$)




exp. @ RCNP



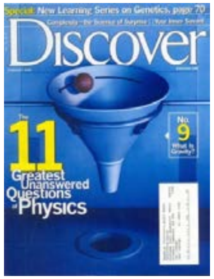




- ✓ GTR excitation energies can be reproduced in a fully self-consistent way.
- ☐ New and most important ingredient: **Fock terms** in CDFT

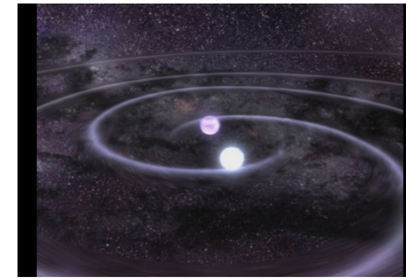
HZL, Giai, Meng, *Phys. Rev. Lett.* **101**, 122502 (2008)

# *r*-process nucleosynthesis & nuclear *β* decays

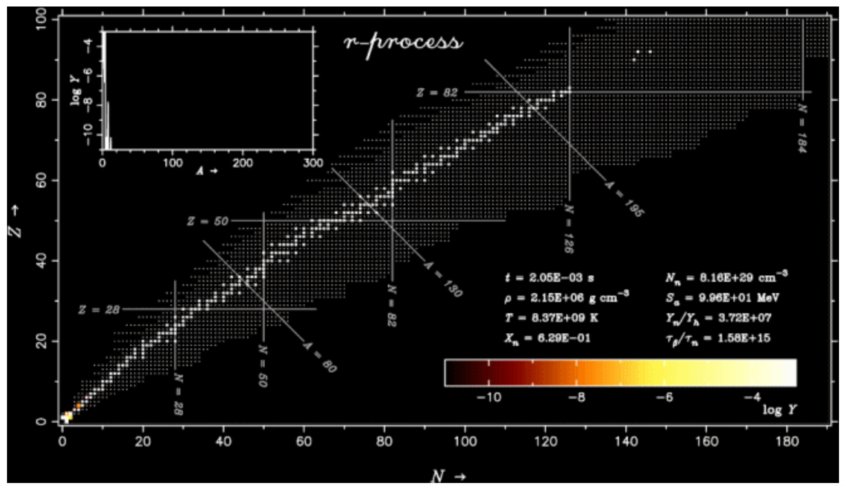
## The 11 greatest unanswered questions of physics




Question 3
How were the heavy elements from iron to uranium made?



**Rapid neutron-capture process (*r*-process)**




Courtesy of S. Wanajo

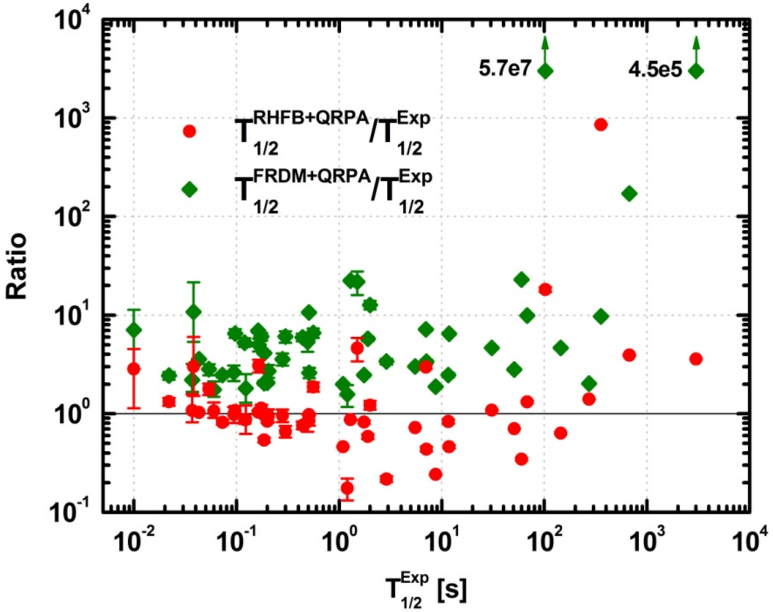
- Nuclear masses ➔ path of *r*-process
- Nuclear *β*-decay rates ➔ timescale of *r*-process

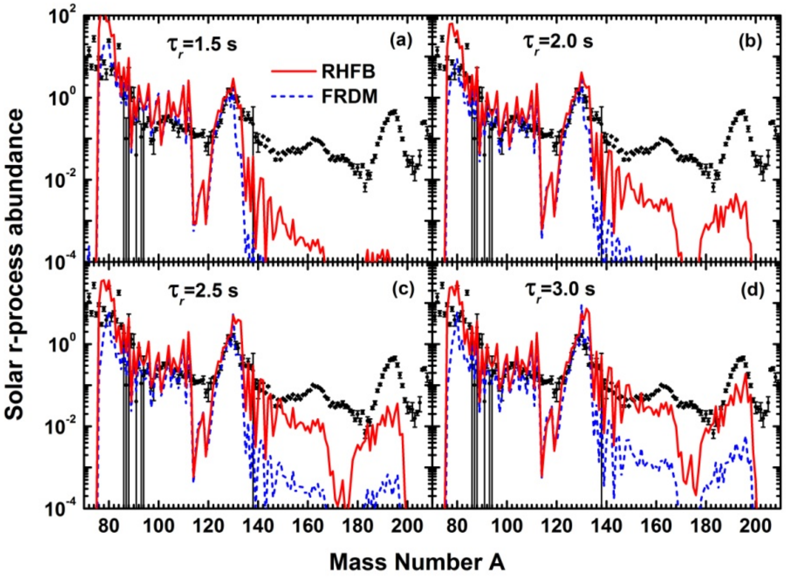
Key exp. @ RIKEN

- EURICA project is providing lots of new *β*-decay data towards *r*-process path.

# $\beta$ decays and $r$-process

**Nuclear $\beta$-decay rates and $r$-process flow** ($Z$ = 20 ~ 50 region)




FRDM+QRPA: widely used nuclear input

RHFB+QRPA: our results

Niu, Niu, HZL, Long, Niksic, Vretenar, Meng, *Phys. Lett. B* **723**, 172 (2013)

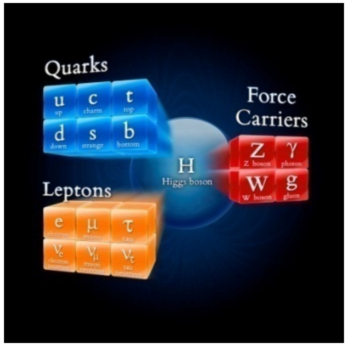
✓ Classical $r$-process calculation shows a faster $r$-matter flow at the $N$ = 82 region and higher $r$-process abundances of elements with $A$ ~ 140.

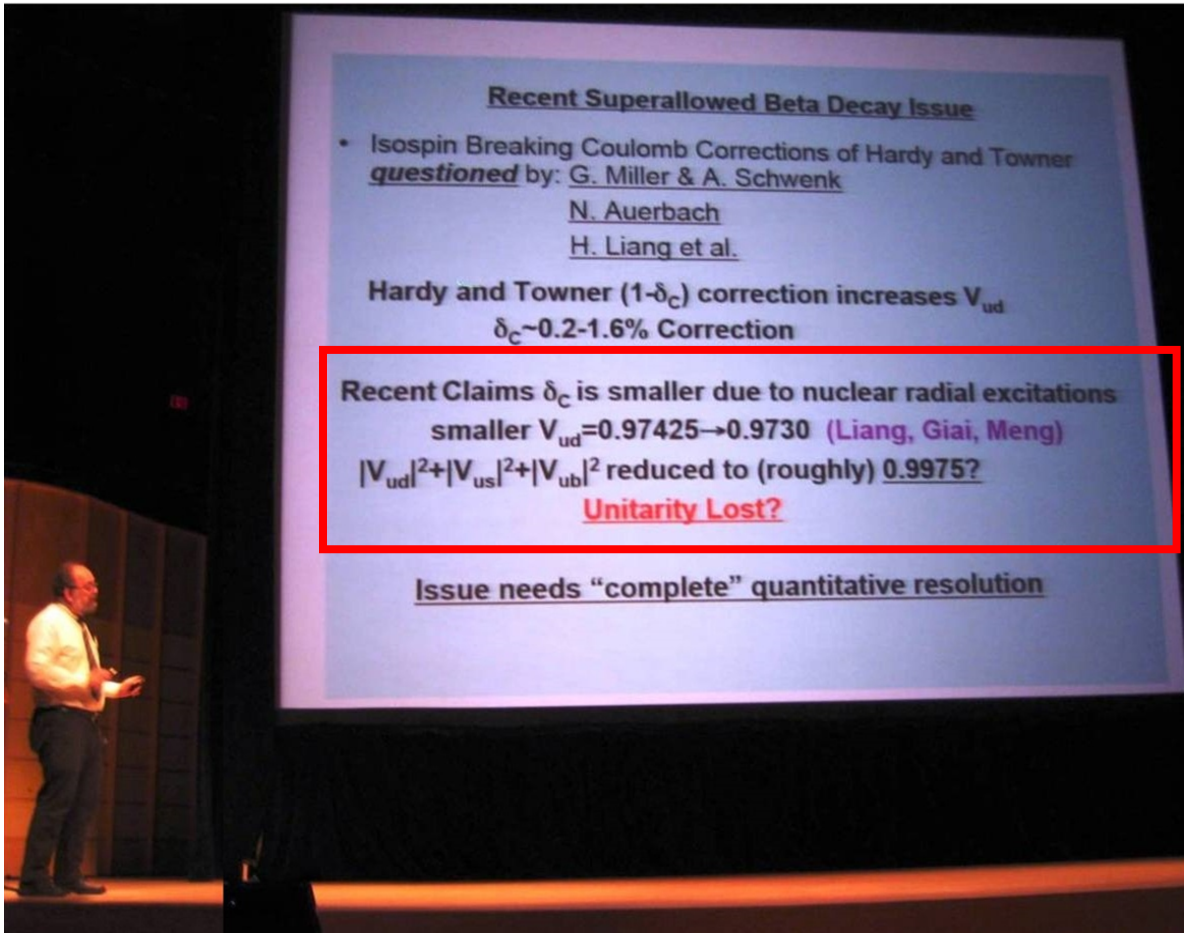
# CKM matrix and its unitarity test

**Cabibbo-Kobayashi-Maskawa matrix**

Nobel Prize 2008

"There exist *at least* three families of quarks in nature."
"Only three?"




Plenary talk in INPC2010 "Precision Electroweak Tests of the Standard Model" by Professor William Marciano

# CKM matrix and its unitarity test

## Cabibbo-Kobayashi-Maskawa matrix

- quark eigenstates of weak interaction ⟺ quark mass eigenstates
- unitarity of CKM matrix ⟺ test of Standard Model

$$\begin{pmatrix} |V_{ud}| & |V_{us}| & |V_{ub}| \\ |V_{cd}| & |V_{cs}| & |V_{cb}| \\ |V_{td}| & |V_{ts}| & |V_{tb}| \end{pmatrix} = \begin{pmatrix} 0.97425 \pm 0.00022 & 0.2252 \pm 0.0009 & 0.00415 \pm 0.00049 \\ 0.230 \pm 0.011 & 1.006 \pm 0.023 & 0.0409 \pm 0.0011 \\ 0.0084 \pm 0.0006 & 0.0429 \pm 0.0026 & 0.89 \pm 0.07 \end{pmatrix}$$

## Unitarity test

Particle Data Group 2016

- the most precise test comes from $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2$
- the most precise $|V_{ud}|$ comes from nuclear $0^+ \rightarrow 0^+$ superallowed $\beta$ transitions

## Nuclear superallowed $\beta$ transitions

$$|M_F|^2 = |\langle f|\, T_+ \,|i\rangle|^2 = |M_0|^2(1-\delta_c)$$

- experimental measurements
- theoretical corrections (isospin symmetry-breaking corrections)

# Isospin corrections & $V_{ud}$

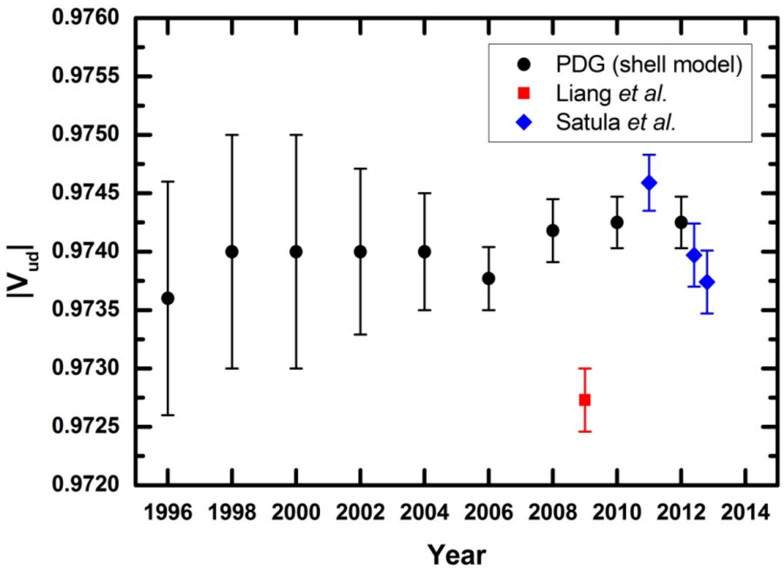
PHYSICAL REVIEW C **79**, 064316 (2009)

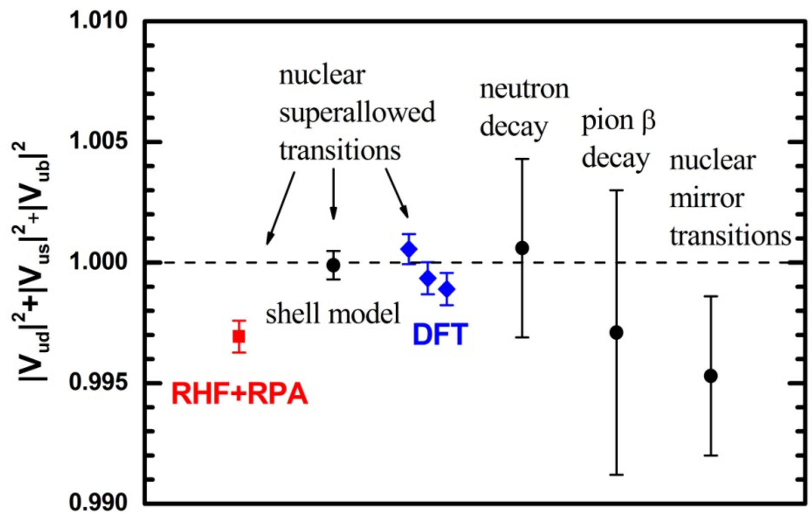
**Isospin corrections for superallowed Fermi $\beta$ decay in self-consistent relativistic random-phase approximation approaches**

Haozhao Liang (梁豪兆),[1,2] Nguyen Van Giai,[2] and Jie Meng (孟杰)[1,3]

cited by PDG 2010, 2012, 2014, ...

## Isospin corrections by self-consistent CDFT



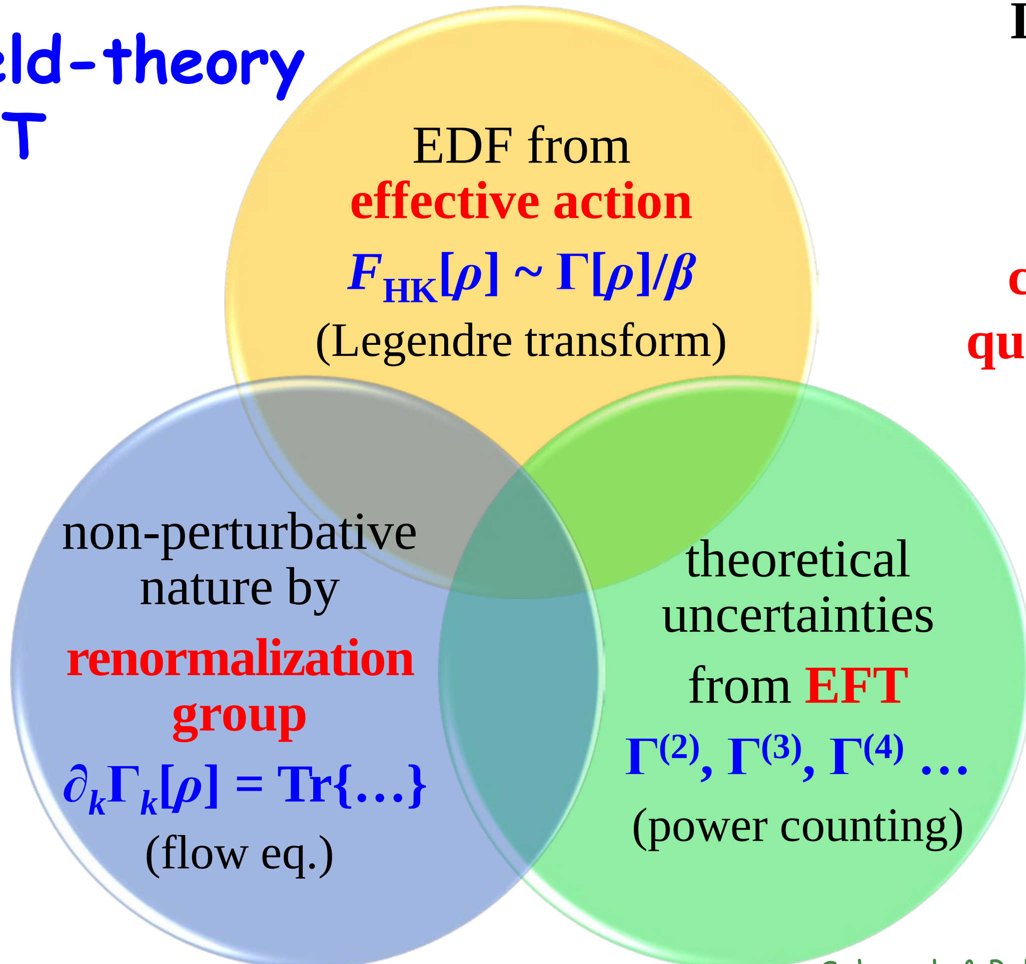




HZL, Giai, Meng, *PRC* **79**, 064316 (2009); Satula *et al.*, *PRL* **106**, 132502 (2011); *PRC* **86**, 054316 (2012)

- To our best knowledge: $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2$: **0.997 ~ 1.000** (**the 4$^{th}$ family?**)
- ongoing studies ……

# A dream for next-generation DFT

**quantum-field-theory oriented DFT**




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


IUPAP Young Scientist Prize
@ INPC2016, Australia

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 $\boldsymbol{\rho(\mathbf{x})}$.

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

- ✓ There exist **a universal density functional** $F_{\mathrm{HK}}[\rho(\mathbf{x})]$.
- ✓ The ground-state energy $E_{\mathrm{gs}}$ 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 $\boldsymbol{U(\mathbf{x})}$.

# EDF from effective action

**Strategy:** $F_{HK}[\rho] \leftarrow \Gamma[\rho] \leftarrow$ **partition function** $\leftarrow$ **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**

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

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

- **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** $F_{\mathrm{HK}}[\rho]$ 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**

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

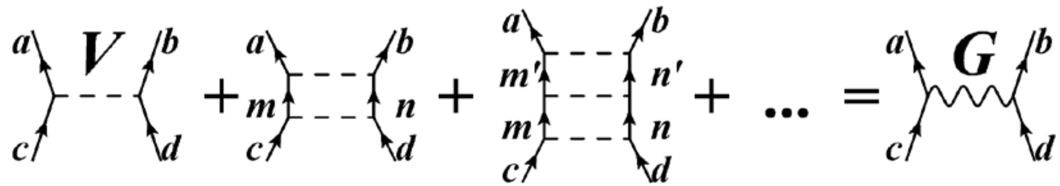
*proof*

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

# 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)



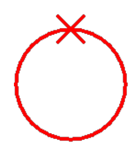

- **Functional Renormalization Group (FRG)** --- Wetterich, *PLB* **301**, 90 (1993)

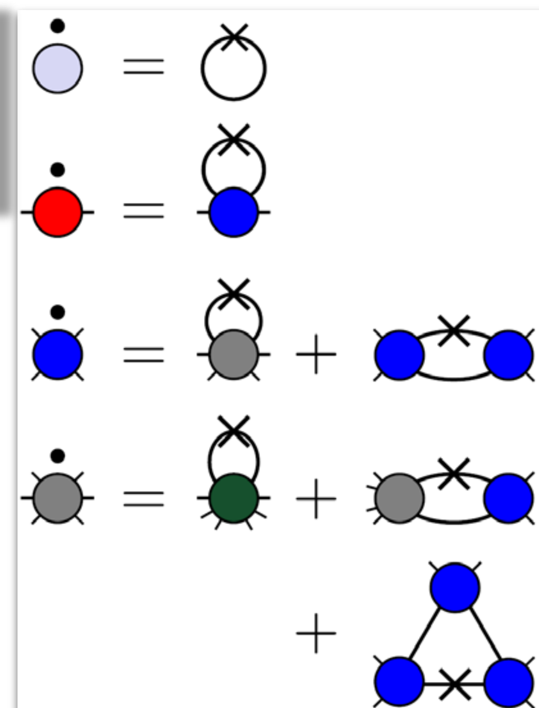
**Exact evolution equation for the effective potential**

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

***Flow equation***

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



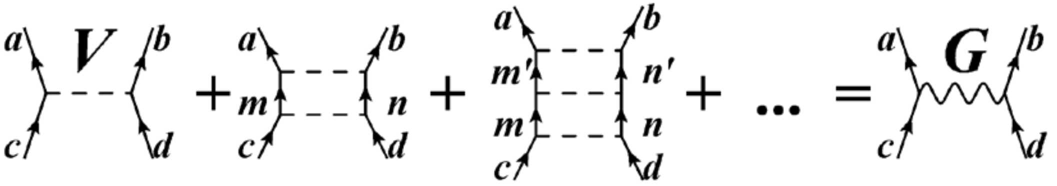


***Cited 1500+ times*** *(google scholar, October 2017)*
***in QCD, hadron, nuclear, cold atom, condensed matter, quantum chemistry ……***

# 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)

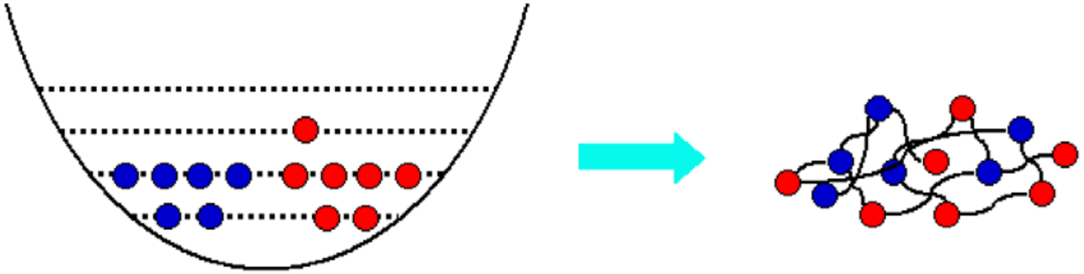



- **Functional Renormalization Group (FRG) ---** Wetterich, *PLB* **301**, 90 (1993)

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

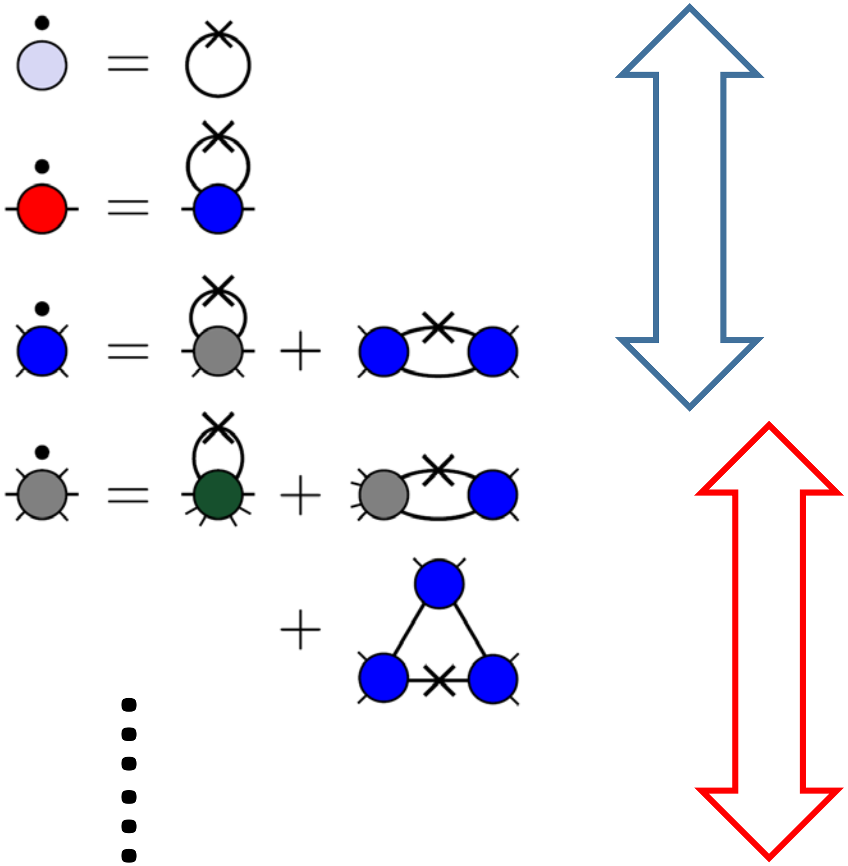
***Flow equation***

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



# Theoretical uncertainty

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



**To solve exactly?**

**To estimate smartly?**

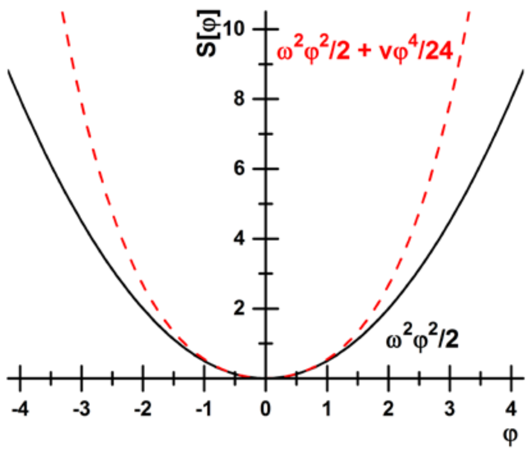
- Proper power counting by **$\Gamma^{(0)}$, $\Gamma^{(2)}$, $\Gamma^{(3)}$, $\Gamma^{(4)}$ …?**
- Controllable theoretical uncertainty**?**

# $\varphi^4$-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 (**$v_0 = v/\omega^4$**)

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

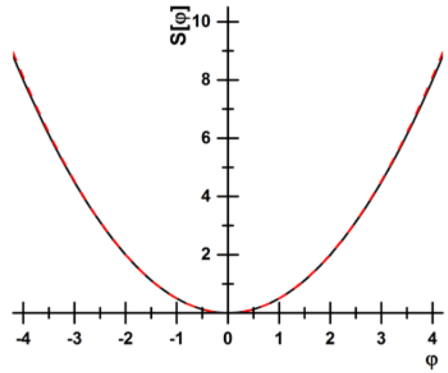
- Ground-state density

$$\rho_{\mathrm{gs}} = \langle\varphi^2\rangle = \frac{1}{Z}\frac{\delta Z[J]}{\delta J}\bigg|_{J=0}$$

$$= \frac{1}{\omega^2}\left[\frac{3}{2}K_{\frac{5}{4}}\left(\frac{3}{4v_0}\right) + \frac{3}{2}K_{-\frac{3}{4}}\left(\frac{3}{4v_0}\right) - (v_0+3)K_{\frac{1}{4}}\left(\frac{3}{4v_0}\right)\right] \Big/ \left[v_0 K_{\frac{1}{4}}\left(\frac{3}{4v_0}\right)\right]$$

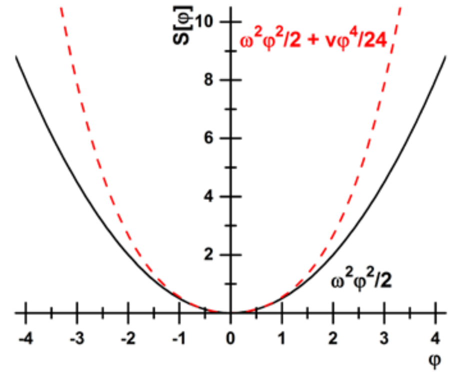
# Typical cases

**$v/\omega^4 = 0.01$**



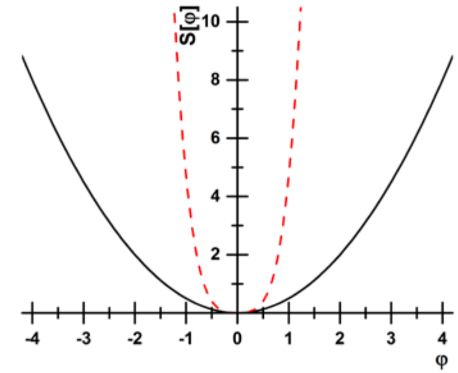

**perturbative**

**$v/\omega^4 = 1$**

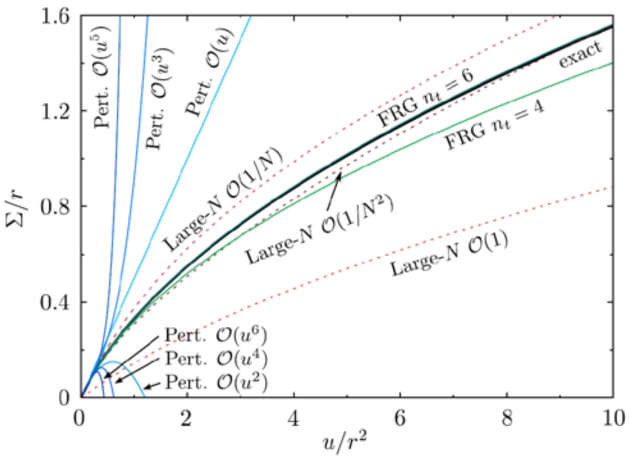


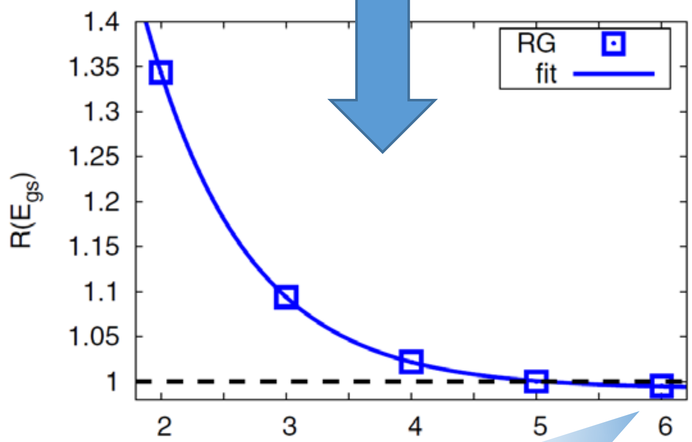

**non-perturbative**

**$v/\omega^4 = 100$**




**highly non-perturbative**




**barely discussed**

**2% error in $6^{\text{th}}$-order cal.**

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

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

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

# 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**

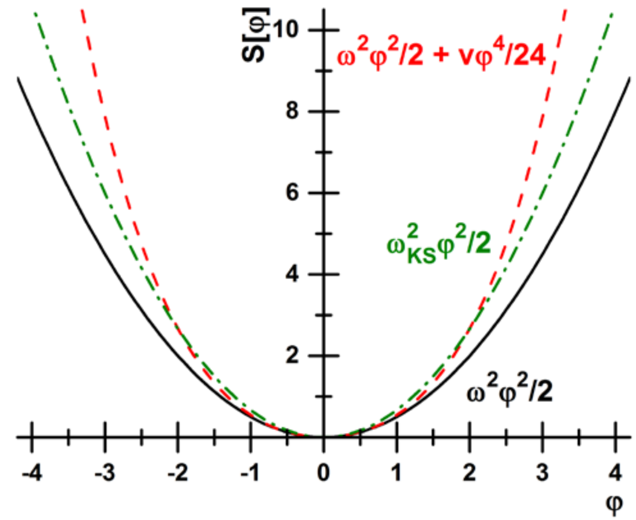
$$\Gamma_\lambda[\rho] = \Gamma_{\mathrm{KS},\lambda}[\rho] + \gamma_\lambda[\rho]$$

  - **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, arXiv:1710.00650

**Ideas of Kohn-Sham**

- To introduce an artificial **non-interacting** system which provides **the same** ground-state density $\rho_{gs}$ 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, $E_x[\rho]$.

# Optimized FRG + DFT

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

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

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

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

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

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

⋮

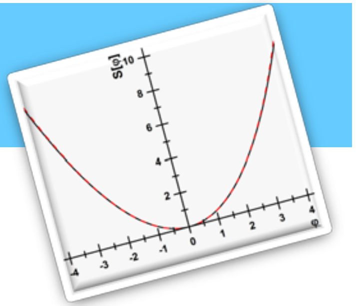
**To solve**

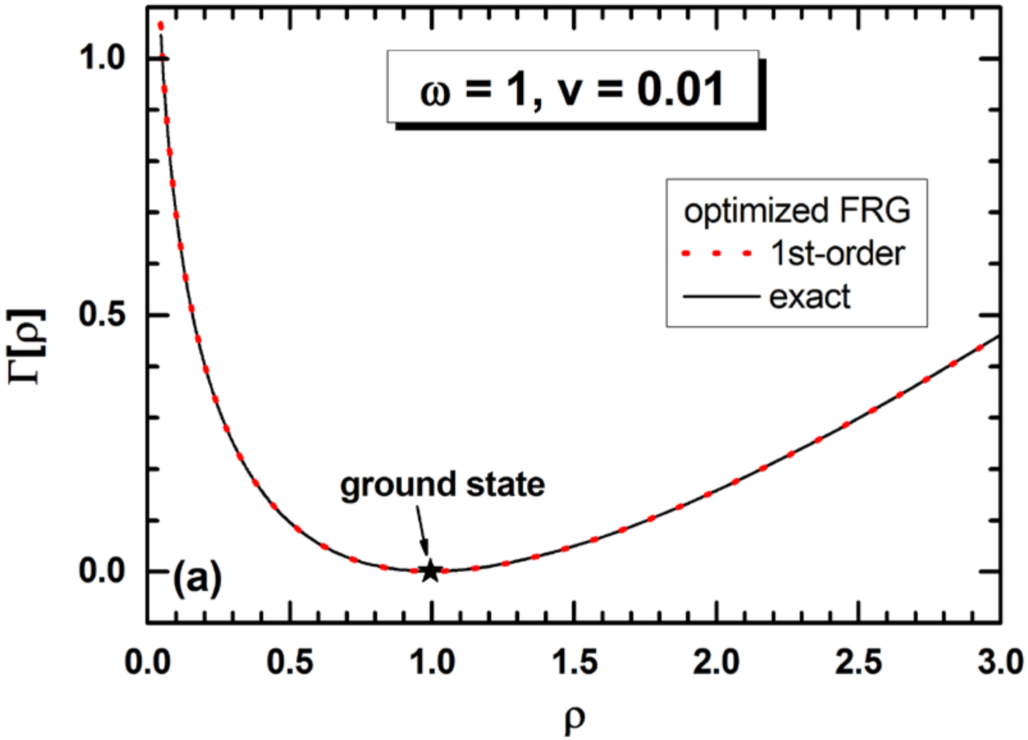
**Estimating upper/lower bounds**

**Keeping as KS counterparts**

# Typical cases (I)

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



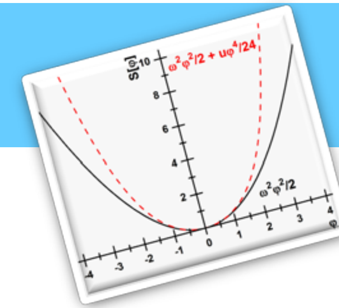



- Effective action vs density, $F_{HK}[\rho]$.

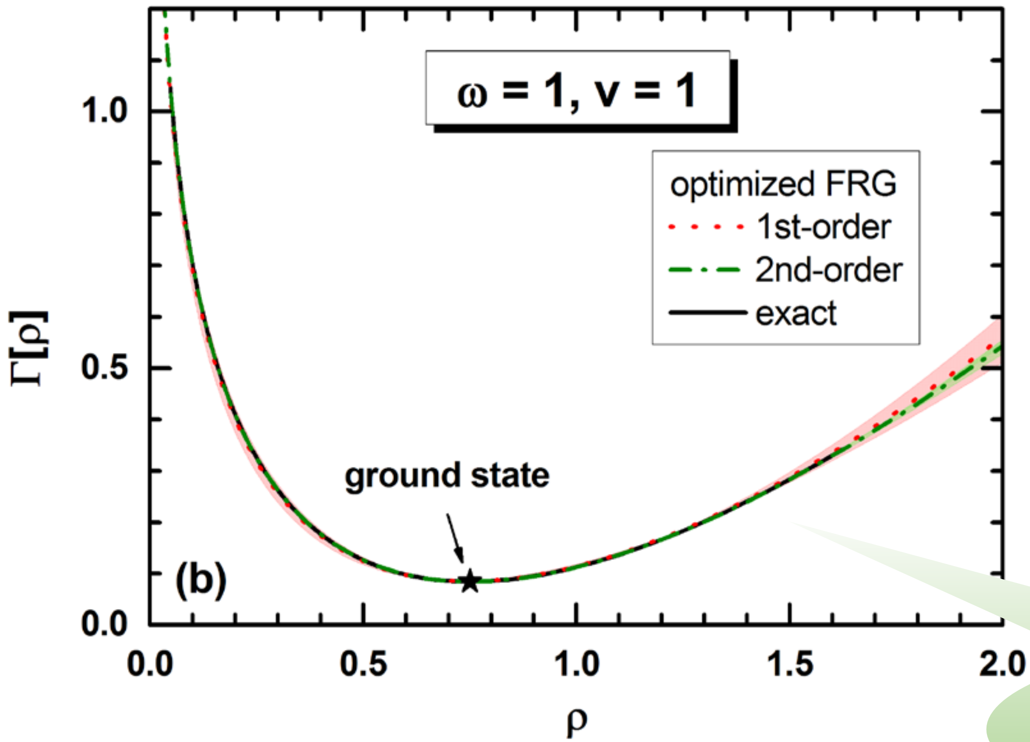
HZL, Niu, Hatsuda, arXiv:1710.00650

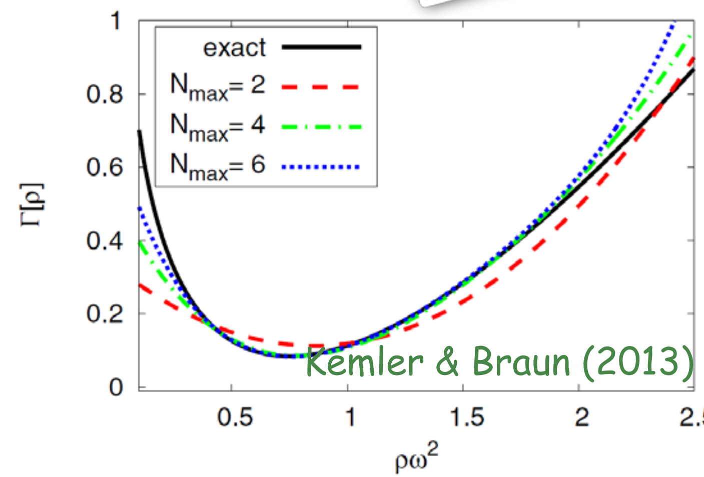
- **1st-order optimized FRG** result is on top of the **exact solution** in a very large density region.
- **Theoretical uncertainty** is invisible in the figure.

# Typical cases (II)



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



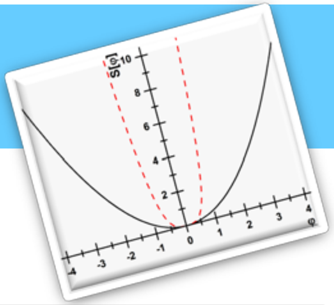




**KS optimized FRG**

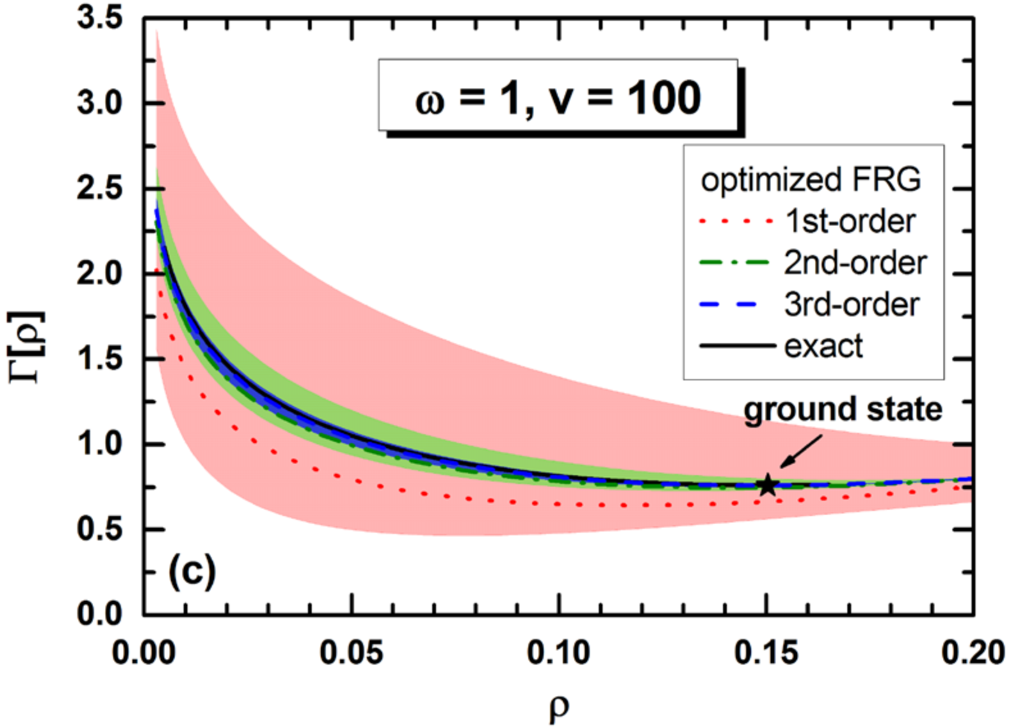
- Effective action vs density, $F_{HK}[\rho]$.

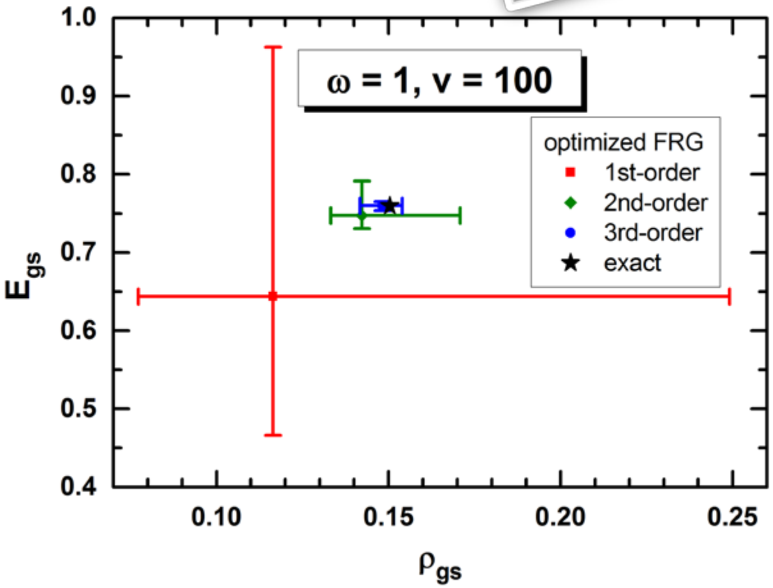
- **1st-order result** reproduces the **exact solution** in a wide density region, with corresponding **uncertainty**.
- **2nd-order result** does improve.

# 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 $\rho_{gs}$ increases by factor **4**, $E_{gs}$ by factor **10** at each order.

# In summary

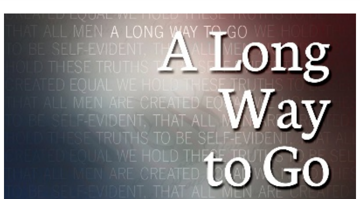
- Ground-state densities and energies: $\varphi^4$-theory in 0D — HZL, Niu, Hatsuda, arXiv:1710.00650

| | $v = 0.01$ | | $v = 1$ | | $v = 100$ | |
|---|---|---|---|---|---|---|
| | $\rho_{\mathrm{gs}}$ | $E_{\mathrm{gs}}$ | $\rho_{\mathrm{gs}}$ | $E_{\mathrm{gs}}$ | $\rho_{\mathrm{gs}}$ | $E_{\mathrm{gs}}$ |
| 1st-order | $0.99506529^{+27}_{-77}$ | $0.001241785^{+55}_{-19}$ | $0.745^{+18}_{-23}$ | $0.0850^{+11}_{-10}$ | $0.12^{+13}_{-4}$ | $0.64^{+32}_{-18}$ |
| 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 | $0.9950653285^{+21}_{-8}$ | $0.001241778944^{+16}_{-44}$ | $0.75052^{+15}_{-15}$ | $0.084529^{+67}_{-68}$ | $0.1482^{+58}_{-65}$ | $0.7597^{+52}_{-62}$ |
| exact | 0.9950653282 | 0.001241778951 | 0.75051 | 0.084557 | 0.1504 | 0.7597 |

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

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

- ✓ EDF $F_{\mathrm{HK}}[\rho]$ 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 $F_{\mathrm{HK}}[\rho]$ are taken into account **order-by-order** with (proper) **theoretical uncertainties**.




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

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|---|---|
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*Thank you!*