

高能与低能核物理交叉学术研讨会
华东师范大学，2026年5月15-18日

探索第一性原理的密度泛函理论

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May 17, 2026



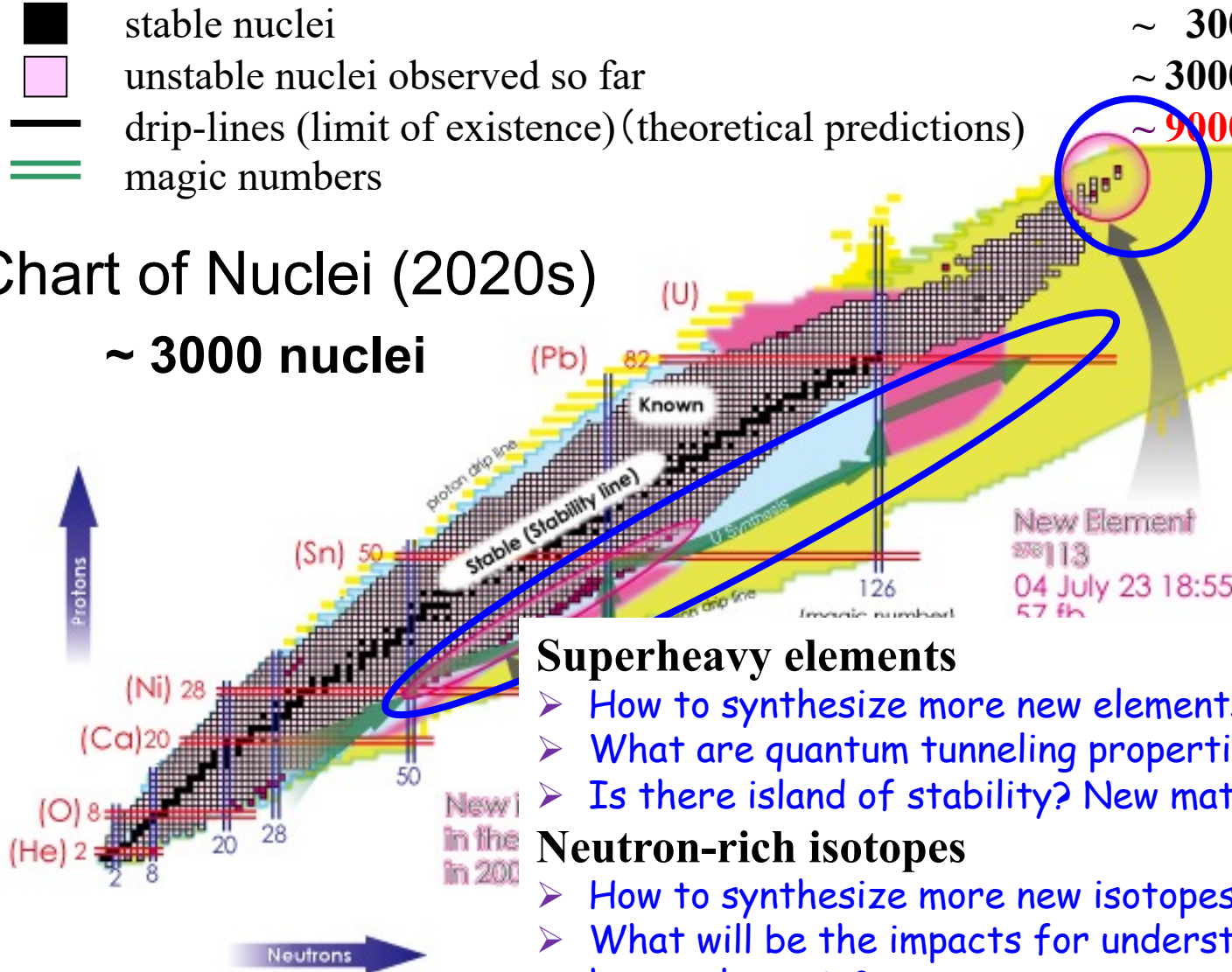
Lab homepage: <http://tnp.phys.s.u-tokyo.ac.jp>

Nuclear chart

- stable nuclei
- unstable nuclei observed so far
- drip-lines (limit of existence) (theoretical predictions)
- == magic numbers

Chart of Nuclei (2020s)

~ 3000 nuclei



~ 300 nuclei
~ 3000 nuclei
~ 9000 nuclei



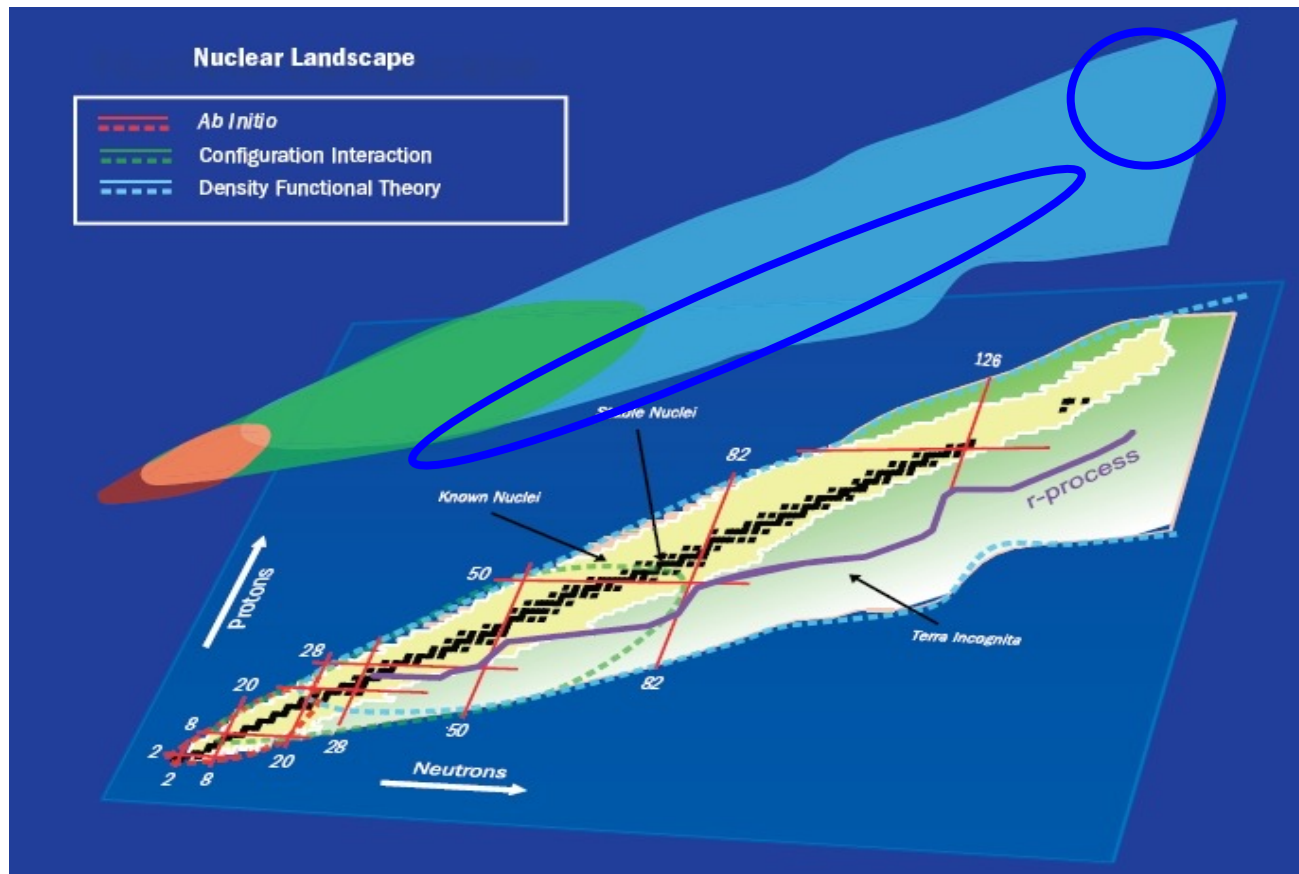
Superheavy elements

- How to synthesize more new elements?
- What are quantum tunneling properties of SHE?
- Is there island of stability? New materials?

Neutron-rich isotopes

- How to synthesize more new isotopes?
- What will be the impacts for understanding origins of heavy elements?
- What will be the impacts for handling nuclear wastes?

state-of-the-art nuclear methodologies



<http://www.unedf.org/>

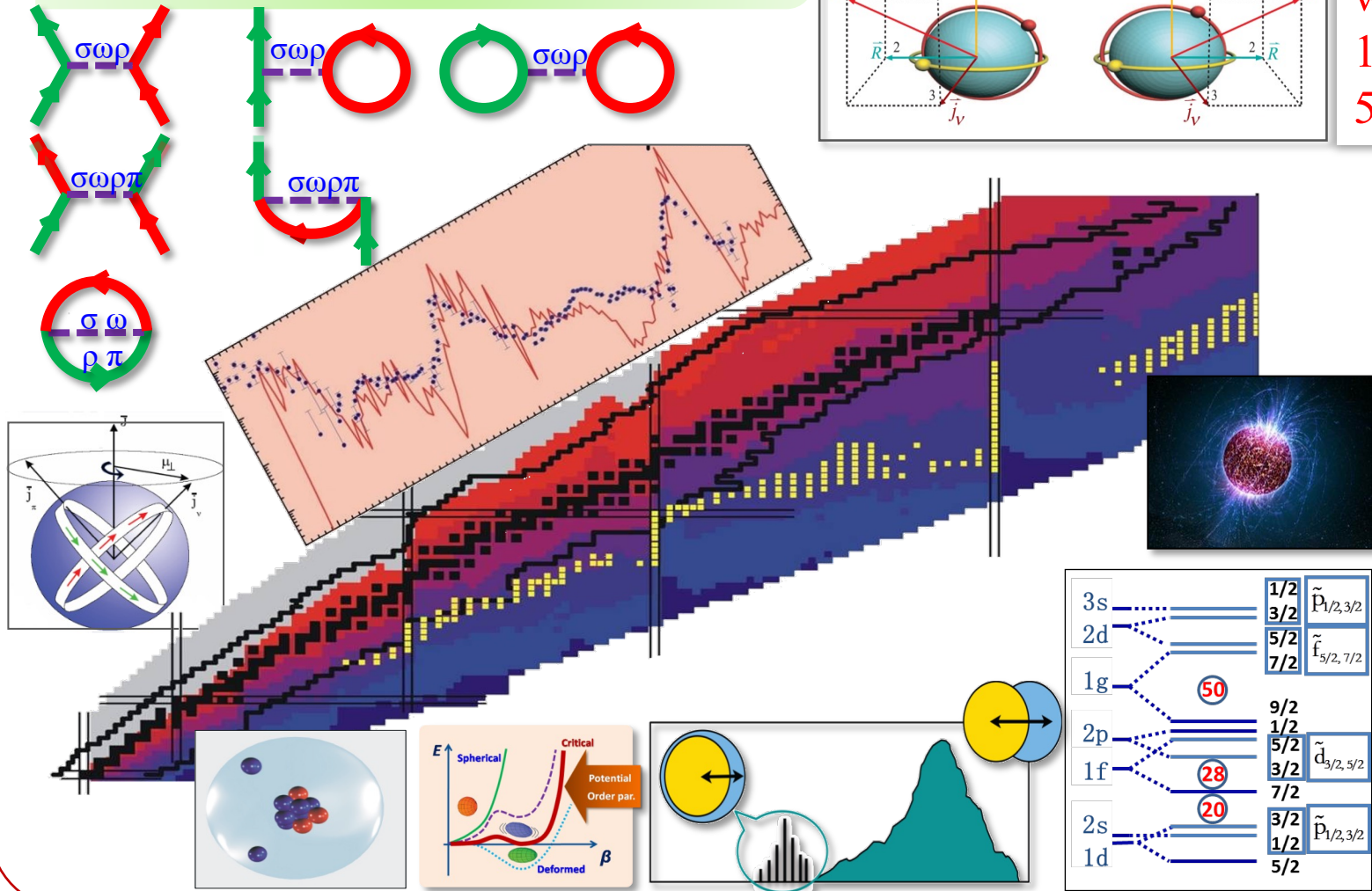
- Density functional theory (DFT) aims at understanding both ground-state and excited-state properties of thousands of nuclei in a consistent and predictive way.

Applications of CDFT

《物理学进展》2011年31卷第4期

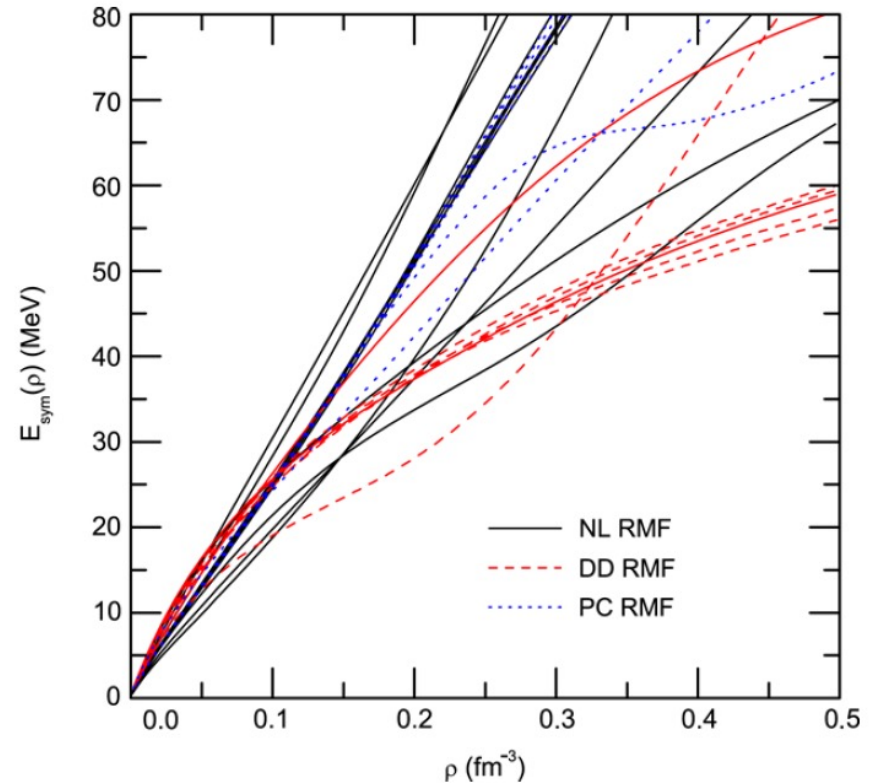
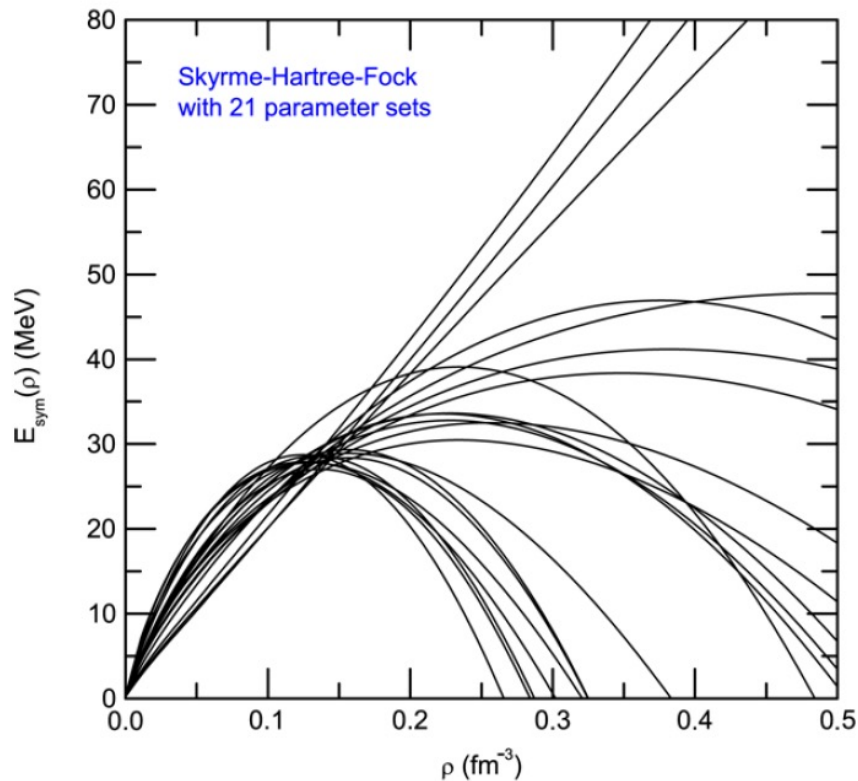
原子核协变密度泛函理论

138 pp
with
122 figs
595 refs



Phenomenological energy density functionals

■ *Predictions of phenomenological energy density functionals (EDF)* (10 years ago)



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

DFT for Coulomb systems

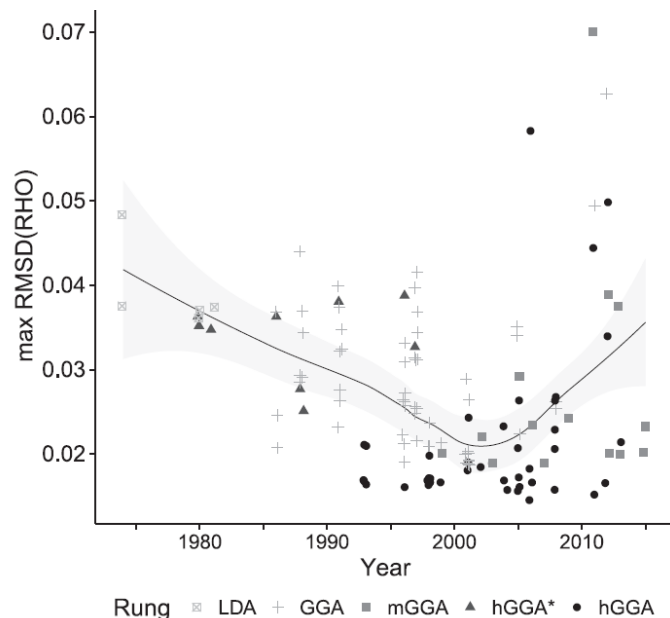
RESEARCH

REPORT

THEORETICAL CHEMISTRY

Density functional theory is straying from the path toward the exact functional

Michael G. Medvedev,^{1,2,3,*†} Ivan S. Bushmarinov,^{1,*†} Jianwei Sun,^{4,†}
John P. Perdew,^{4,5,†} Konstantin A. Lyssenko^{1,†}



RESEARCH

TECHNICAL COMMENT

THEORETICAL CHEMISTRY

Comment on “Density functional theory is straying from the path toward the exact functional”

Kasper P. Kepp

INSIGHTS | PERSPECTIVES

CHEMISTRY

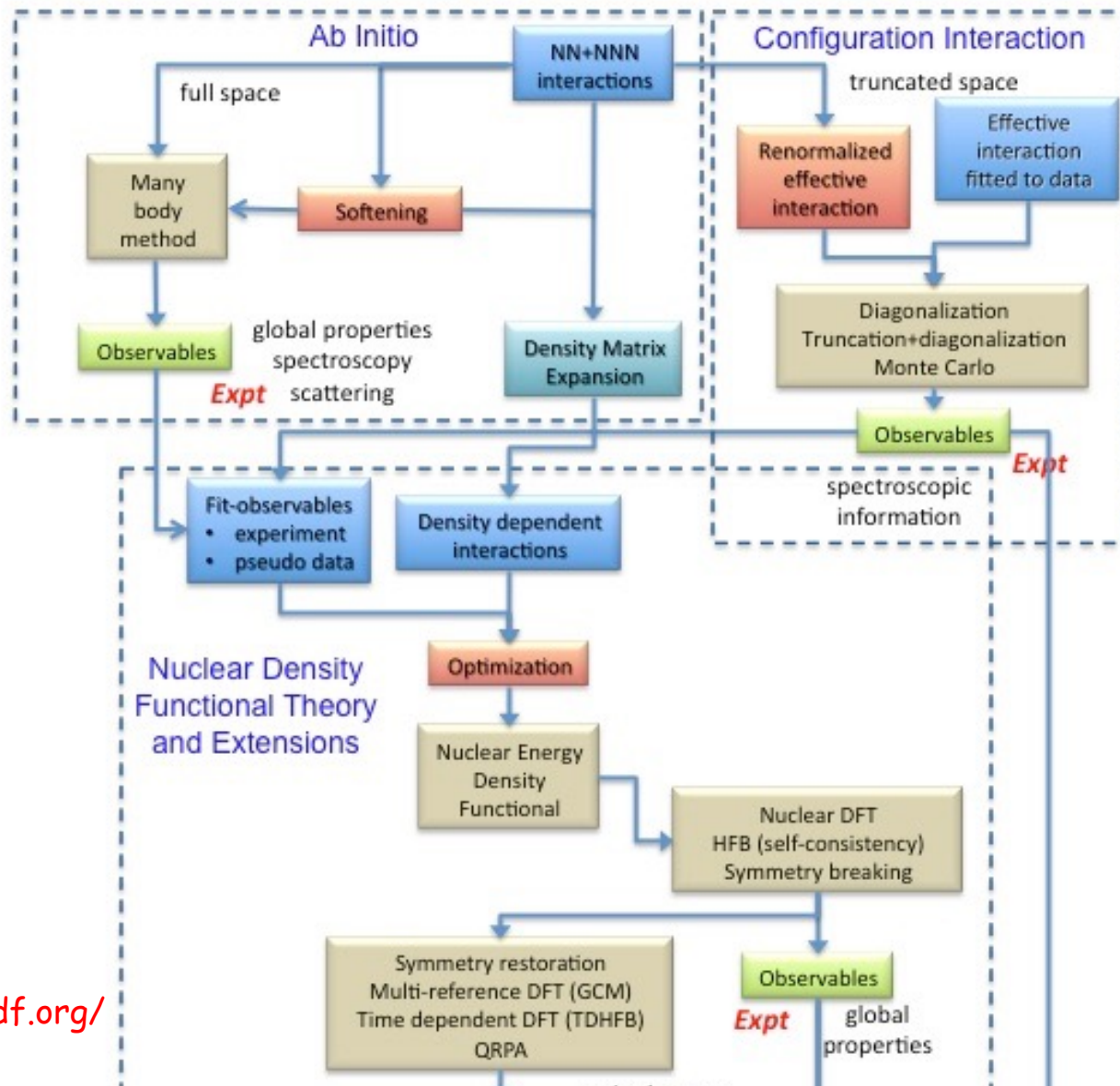
A conundrum for density functional theory

DFT studies may sometimes get the right results for the wrong reasons

Medvedev *et al.*, *Science* 355, 49-52 (2017)
Hammes-Schiffer, *Science* 355, 28-29 (2017)
Kepp, *Science* 356, 496 (2017)

Possible strategies

UNEDF



A review

Invited Review in *Progress in Particle and Nuclear Physics*

Progress in Particle and Nuclear Physics 109 (2019) 103713



Review

Towards an *ab initio* covariant density functional theory for nuclear structure

Shihang Shen^{a,b,c}, Haozhao Liang^{d,e}, Wen Hui Long^{f,g}, Jie Meng^{a,h,i,*},
Peter Ring^{a,j}

53 pages
with 26 figs and 436 references

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)

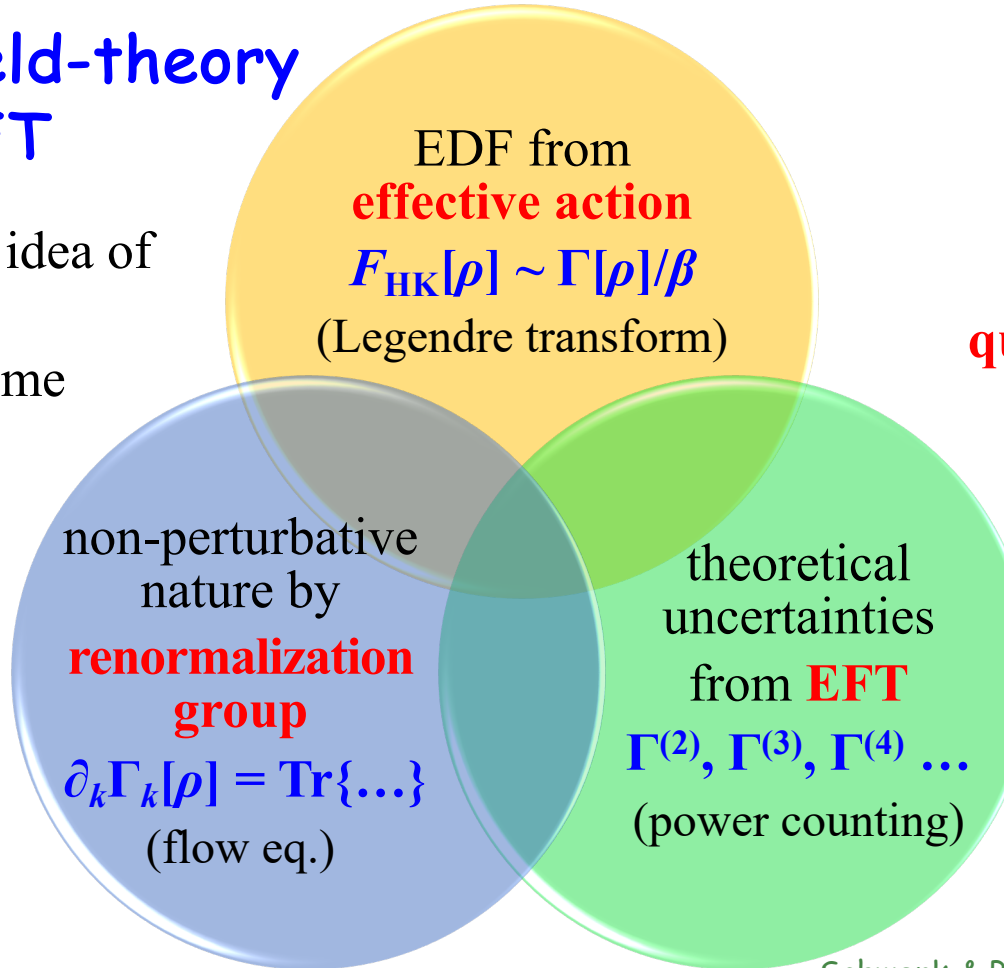
Shen, HZL, Meng, Ring, Zhang, *PLB* **781**, 227 (2018)

quantum-field-theory
oriented DFT

We proposed the idea of
Functional RG +
Kohn-Sham scheme

(KS-FRG)

HZL, Niu, Hatsuda,
PLB 779, 436 (2018)



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

● ● ● ● ● ●



cf. <http://www.unedf.org/>

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)



@ INPC2016, Australia

● ● ● ● ● ●

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** $F_{\text{HK}}[\rho(\mathbf{x})]$.
- ✓ 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

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

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

Where $F_{\text{HK}}[\rho(\mathbf{x})] = \min_{\Psi_{\rho}} \langle \Psi_{\rho} | \hat{T} + \hat{V} | \Psi_{\rho} \rangle$ 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: $F_{\text{HK}}[\rho] \leftarrow \Gamma[\rho] \leftarrow \text{partition function} \leftarrow \text{path integral}$

□ Classical action in Euclidean space

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

where $U(\mathbf{x})$ is one-body potential and $V(\mathbf{x}_1, \mathbf{x}_2)$ is two-body interaction.

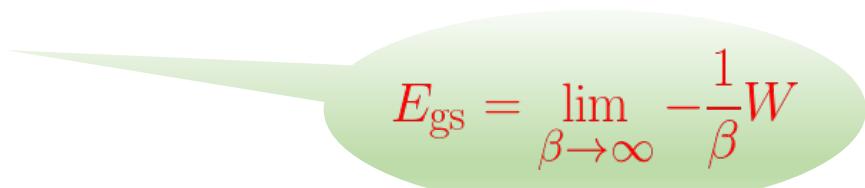
□ Partition function in two-particle point-irreducible (**2PPI**) scheme

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

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

□ Thermodynamic potential / generating function / Schwinger function

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


$$E_{\text{gs}} = \lim_{\beta \rightarrow \infty} -\frac{1}{\beta} W$$

Connection to Hohenberg-Kohn theorem

□ Local density

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

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

□ Effective action $\leftarrow$ Legendre transform of W with respect to J

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

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

Second Legendre transform $\rightarrow$ HK theorem

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

proof

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

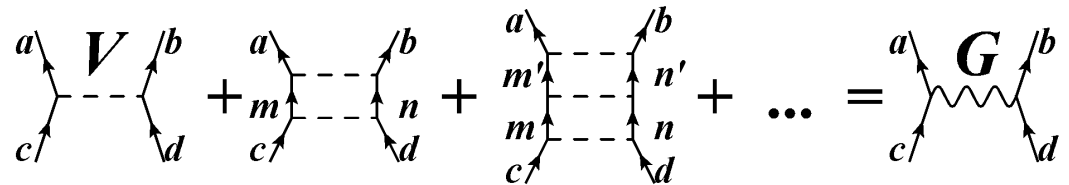
Non-perturbative nature of interaction

□ Lippmann-Schwinger eq. / Bethe-Goldstone eq. / Brueckner theory

Brueckner Hartree-Fock, hole-line expansion ... (in 1960s, 70s)

Relativistic BHF for finite nuclei

Shen, HZL, Long, Meng, Ring,
PPNP 109, 103713 (2019).



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

Exact evolution equation for the effective potential

Christof Wetterich

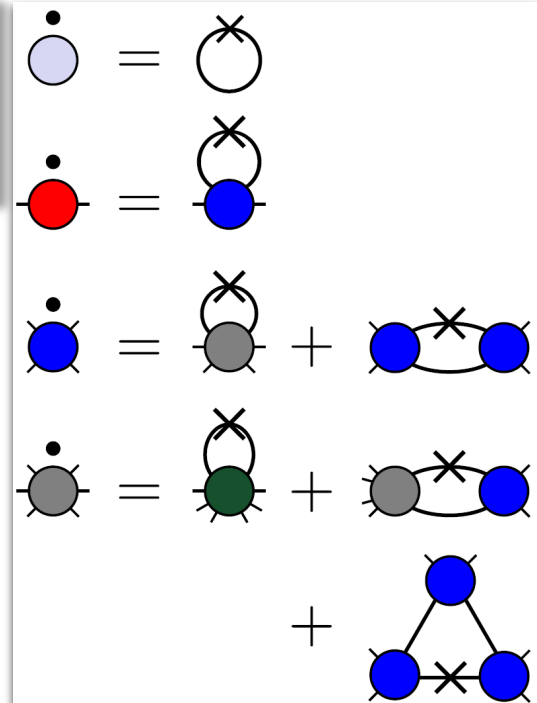
Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, W-6900 Heidelberg, FRG

Flow equation

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

Cited 2800+ times (Google Scholar, Jan 2026)

in QCD, hadron, nuclear, cold atom, condensed matter,
quantum chemistry



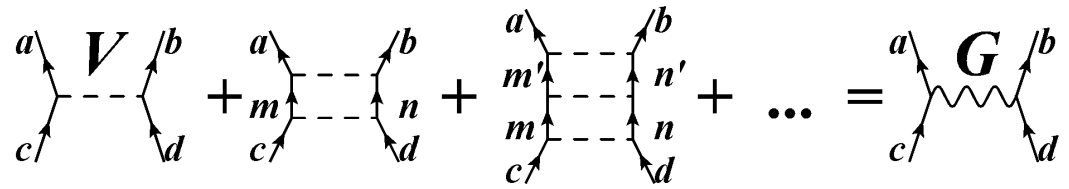
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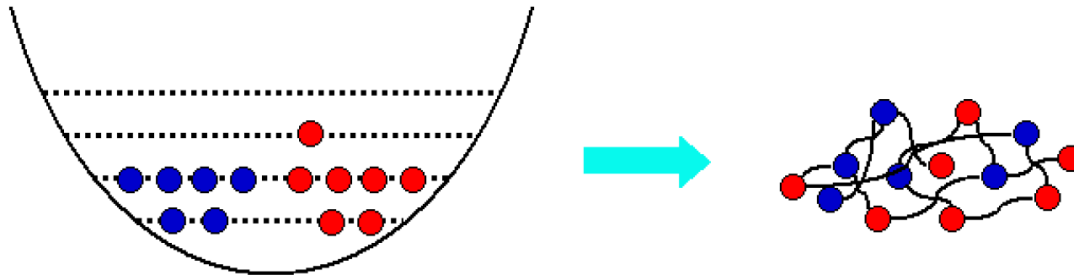


□ Functional Renormalization Group (FRG) --- Wetterich, PLB 301, 90 (1993)

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

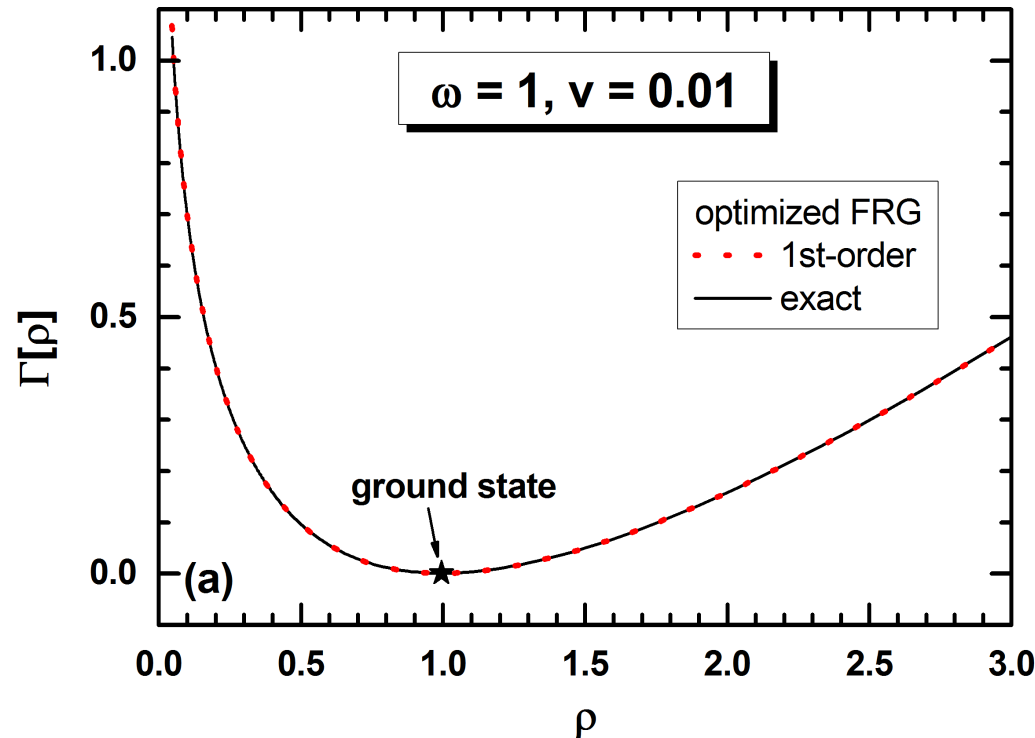
Flow equation

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



ϕ^4 -theory in zero dimension

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



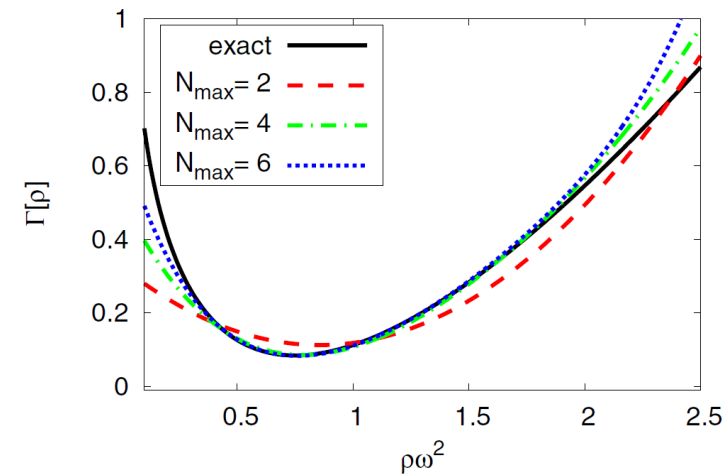
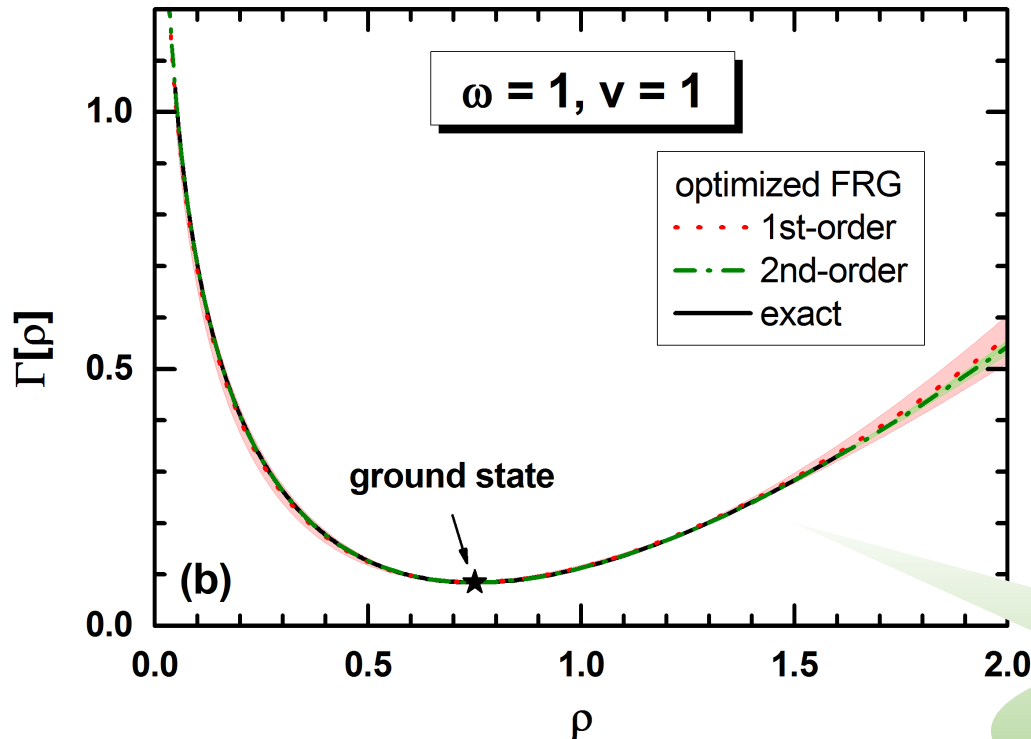
◆ Effective action *vs* density, $F_{\text{HK}}[\rho]$. HZL, Niu, Hatsuda, *Phys. Lett. B* 779, 436 (2018)

□ **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.

ϕ^4 -theory in zero dimension

□ Non-perturbative case $v_0 = v/\omega^4 = 1$ HZL, Niu, Hatsuda, *Phys. Lett. B* 779, 436 (2018)



Kemler & Braun, *JPG* 40, 085105 (2013)

KS optimized FRG

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

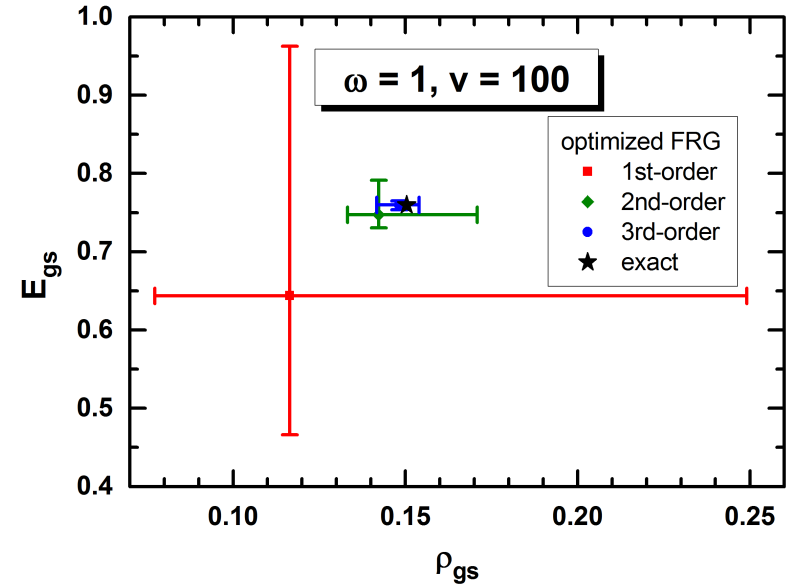
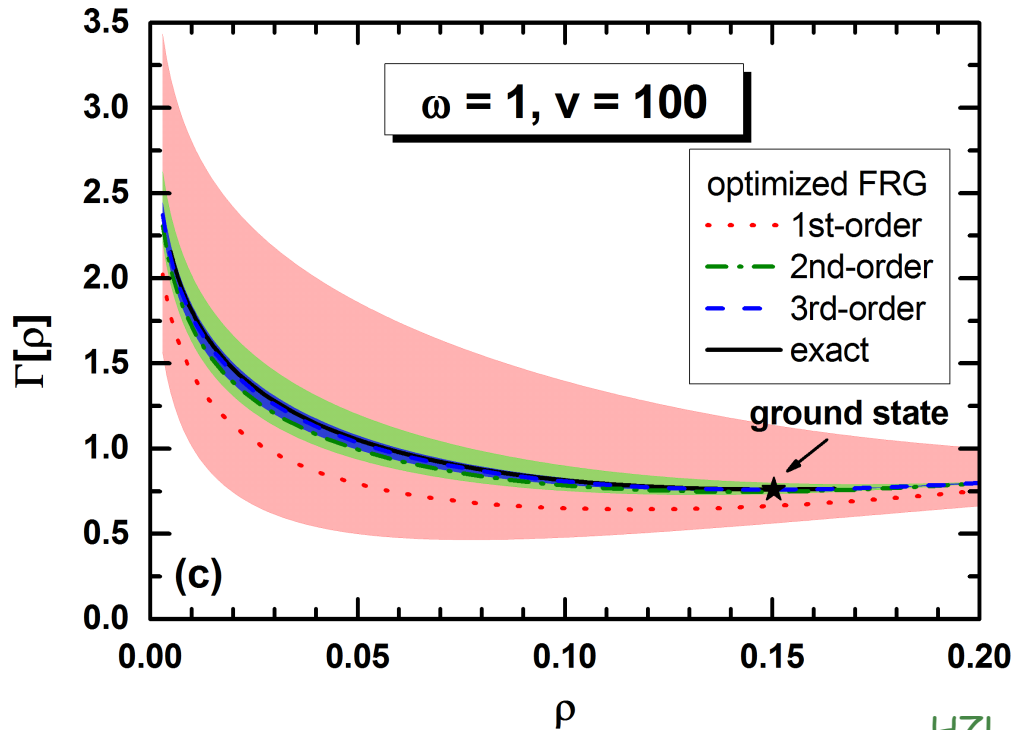
□ 1st-order result reproduces the exact solution in a wide density region, with corresponding uncertainty.

□ 2nd-order result does improve.

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

ϕ^4 -theory in zero dimension

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



◆ Ground-state density and energy.

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

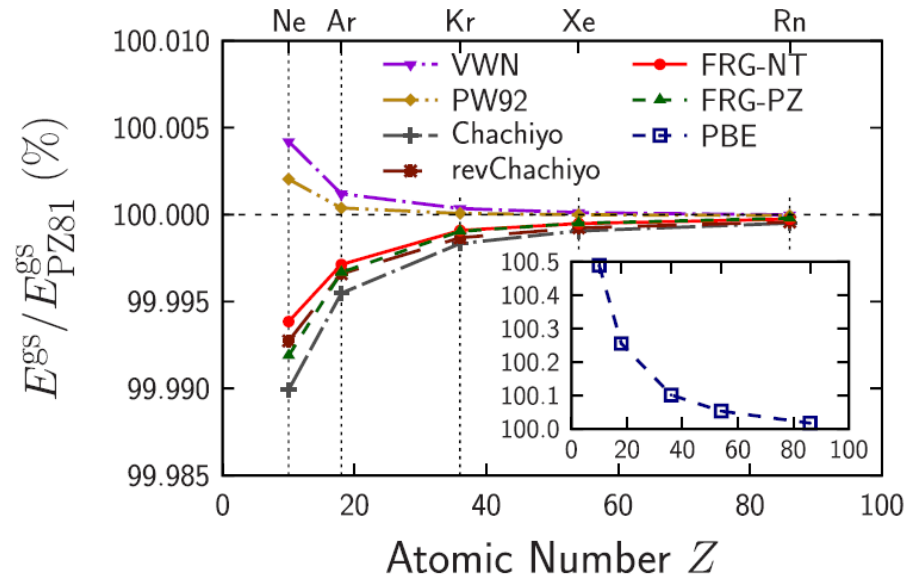
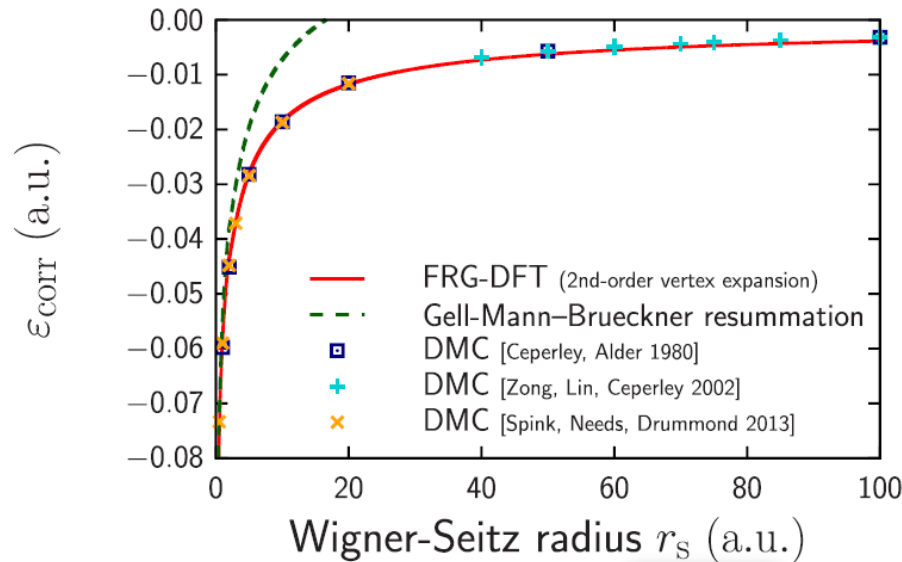
□ 1st-order result is still able to describe the exact solution with large uncertainty.

□ 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.

Progress in 3D electron systems

- ◆ Correlation energy of 3D electron gas
- ◆ Ground-state energies of Ne, Ar, Kr, Xe, and Rn atoms



Yokota & Naito, *Phys. Rev. Research* **3**, L012015 (2021).

$$F_{\text{HK}}[\rho] = T_0[\rho] + E_{\text{H}}[\rho] + \underbrace{E_{\text{x}}^{\text{LDA}}[\rho] + E_{\text{c}}^{\text{LDA}}[\rho]}_{\text{ongoing}} + E_{\text{xc}}^{\text{GGA}}[\rho, |\nabla\rho|] + E_{\text{xc}}^{\text{Meta-GGA}}[\rho, |\nabla\rho|, \nabla^2\rho, \tau] + \dots$$

□ Solvable systems?

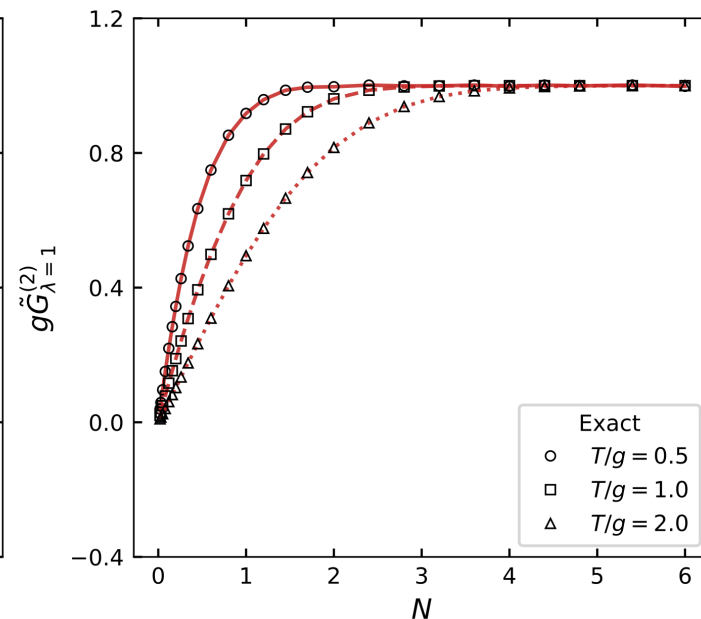
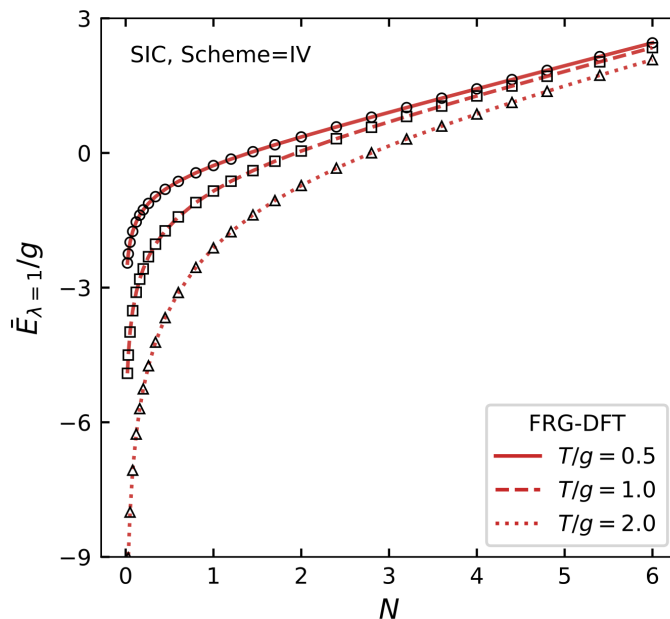
ongoing

- Bose-Hubbard or Fermion-Hubbard models
- 1D interacting bosons or fermions

Single-site Bose-Hubbard model

$$\partial_\lambda \bar{E}_\lambda = \frac{g}{2} N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{N_0} \frac{1}{\beta} \tilde{G}_\lambda^{(2)} \quad \partial_\lambda \mu_\lambda = g N_0 - \frac{g}{2} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \tilde{G}_\lambda^{(3)}$$

$$\partial_\lambda \tilde{G}_\lambda^{(2)} = -g \left(\tilde{G}_\lambda^{(2)} \right)^2 - \frac{g}{2} \frac{1}{\beta} \tilde{G}_\lambda^{(4)} + \frac{g}{2} \frac{1}{\tilde{G}_\lambda^{(2)}} \frac{1}{\beta} \left(\tilde{G}_\lambda^{(3)} \right)^2$$



□ The exact results can be reproduced with the maximum entropy closure.

Wang, Degen, and HZL, in preparation

Samuel Degen (UCLA): American Physical Society's 2025 Steven Chu Award for Best Undergraduate Research (1st Prize)

<https://engage.aps.org/fws/honors/prizes-awards>

Quasi-1D dipolar Fermi gas

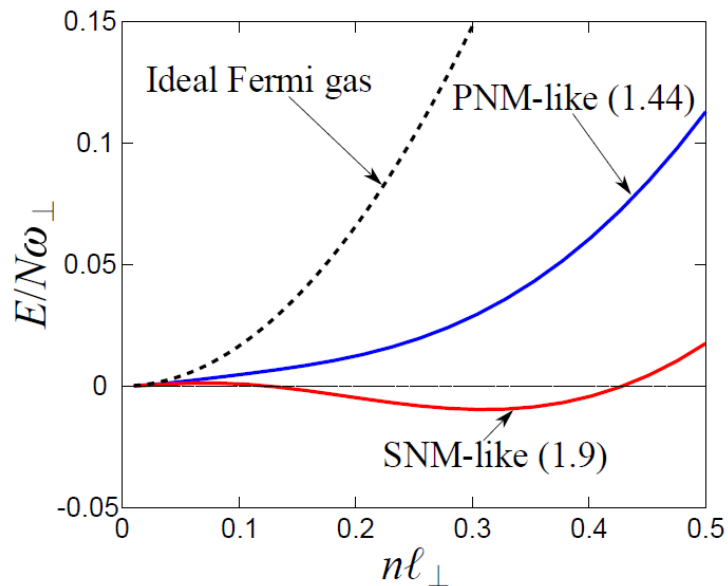
➤ Hamiltonian

$$H = \sum_k \xi_k c_k^\dagger c_k + \frac{1}{2} \sum_{k,k',q} V_{dd}(q) c_k^\dagger c_{k'+q}^\dagger c_{k'} c_{k+q},$$

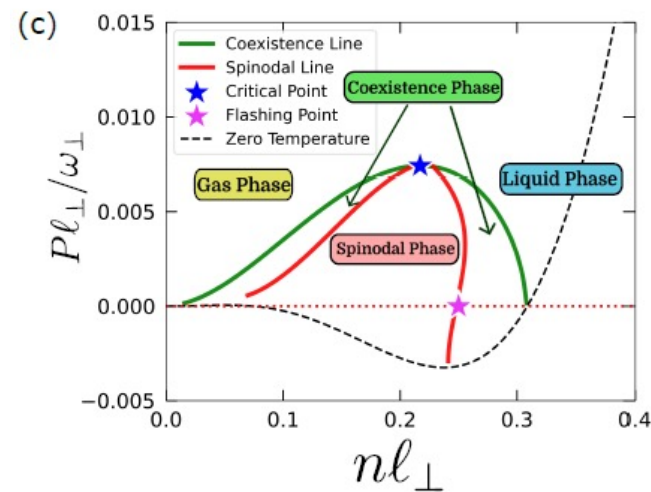
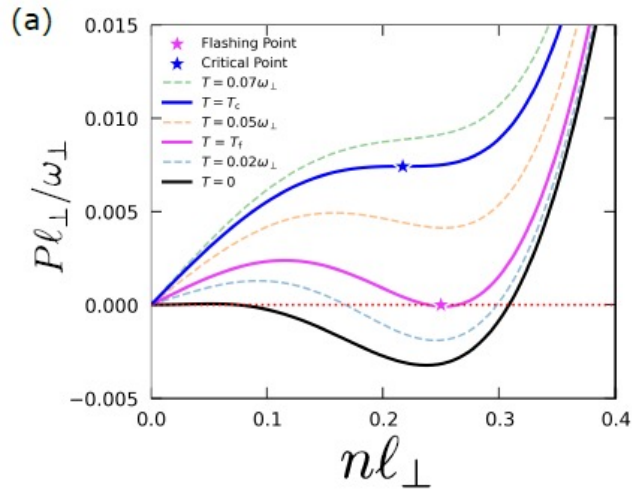
with

$$V_{dd}(q) = -\frac{2\alpha\ell_{dd}}{m\ell_\perp^2} [1 - \sigma_\perp e^{\sigma_\perp} \Gamma(0, \sigma_\perp)],$$

◆ Equation of state ($T = 0$)



◆ Phase transitions (PT) with finite T



PT properties ➔ effective models (Jaqaman or Kapusta) ➔ nuclear matter

1D three-color fermions

PHYSICAL REVIEW LETTERS **135**, 042701 (2025)

Tripling Fluctuations and Peaked Sound Speed in Fermionic Matter

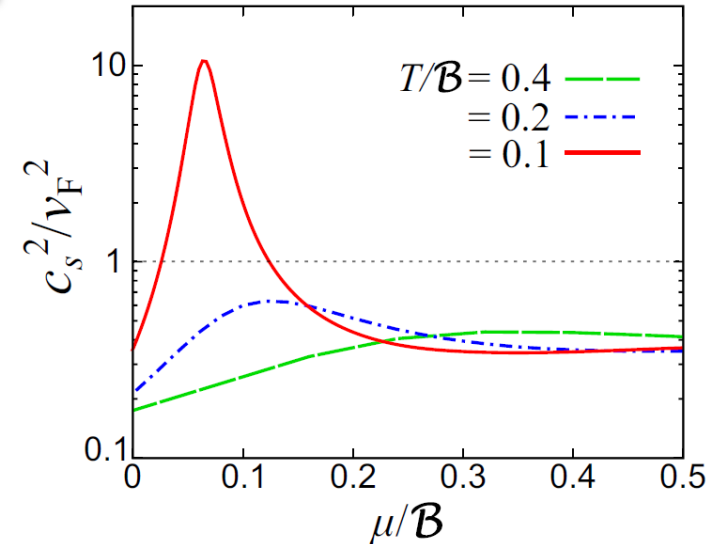
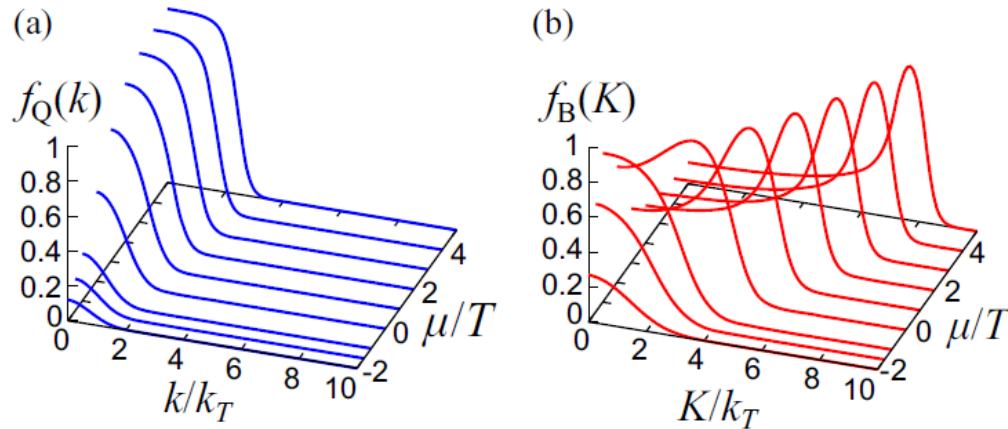
Hiroyuki Tajima^{1,2,3}, Kei Iida^{4,2,5}, Toru Kojo⁶, and Haozhao Liang^{1,7,3}

also see:

Drut et al., *PRL* **120**, 243002 (2018)

McLerran & Reddy, *PRL* **122**, 122701 (2019)

Fujimoto, Kojo, McLerran, *PRL* **132**, 112701 (2024)



- ◆ Momentum distributions of constituent (quarklike) fermions and (baryonlike) three-body states.

- ◆ Squared isothermal sound speed.

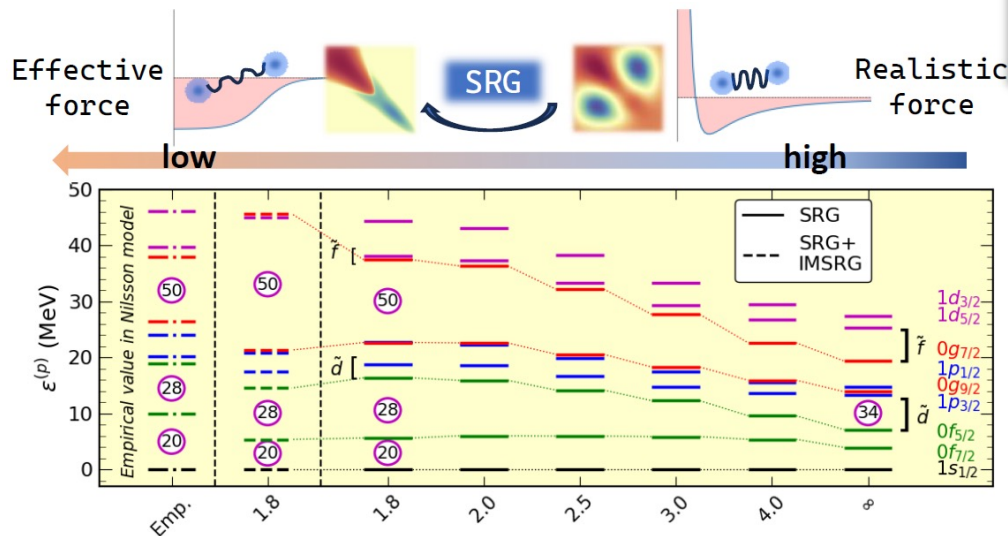
- A crossover involving **three-fermion clusters** is relevant to the **hadron-quark crossover**.
- We examine the role of **tripling fluctuations induced by the formation of three-fermion clusters** by investigating a 1D three-color fermion system analogous to the hadron-quark matter.

From spin to pseudospin symmetry

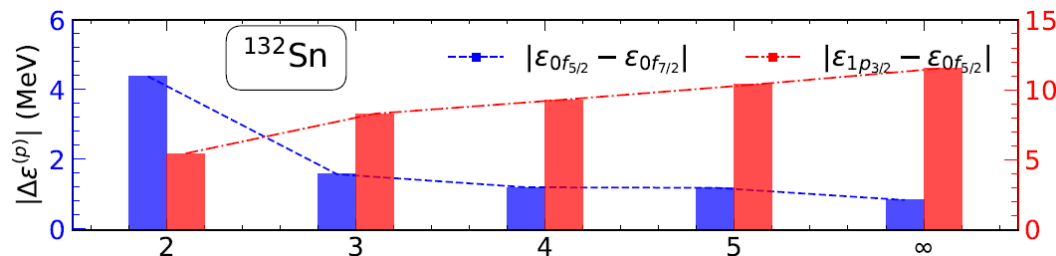
Ding, Wang, Yao, Hergert, HZL, Bogner, *Phys. Rev. Lett.* **136**, 052501 (2026)

Editor's Suggestion & Featured in Physics

◆ HF calculations with SRG and IMSRG forces



◆ RHF calculations



VIEWPOINT

Exposing Nuclear Magic

Vittorio Somà

CEA Paris-Saclay, Gif-sur-Yvette, France

February 2, 2026 • *Physics* 19, 11

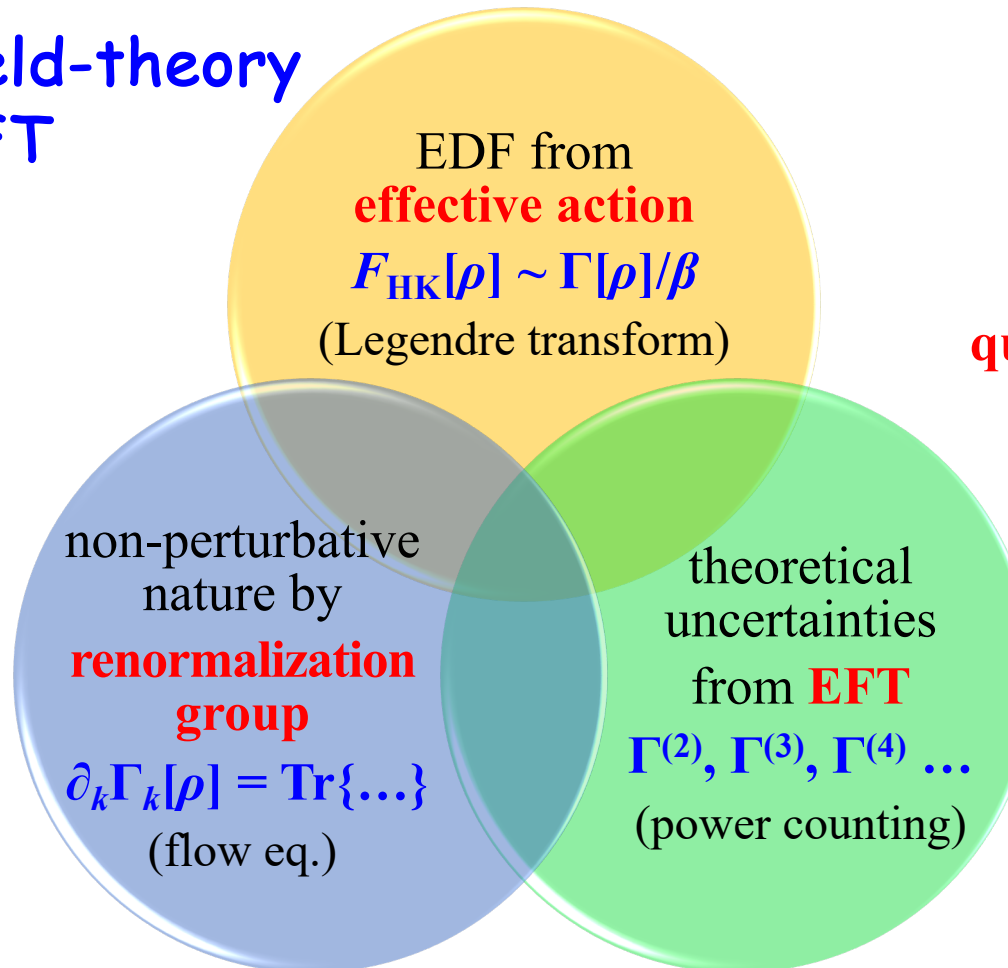
Calculations show how the mysterious “magic numbers” that stabilize nuclear structures emerge naturally from nuclear forces—once these are described with appropriate spatial resolution.



□ A novel transition **from spin to pseudospin symmetry** with decreasing **resolution scale**, accompanied by a **natural emergence of expected magic numbers**.

A dream for new-generation DFT

quantum-field-theory
oriented DFT



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

.....



cf. <http://www.unedf.org/>

Thank you!