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Localized form of Fock terms in nuclear covariant density functional theory

Haozhao Liang （梁豪兆）

RIKEN Nishina Center, Japan

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Original idea

HZL, P.W. Zhao, P. Ring, X. Roca-Maza, J. Meng, *PRC* **86**, 021302(R) (2012)

Outline

Many-body systems and density functional theories

- Research on quantum mechanical many-body problems is essential in many areas of modern physics
  - ⋆ electrons in metal, atoms in molecule, electrons in atom, nucleons in nucleus ...
- Density functional theories (DFT) Hohenberg & Kohn:1964
  - ⋆ reducing the many-body problems formulated in terms of N-particle wave functions to the one-particle level with the local density distribution $\rho(\mathbf{r})$
  - ⋆ no other method achieves comparable accuracy at the same computational cost
- Kohn-Sham scheme Kohn & Sham:1965
  - ⋆ for any interacting system, there exists a **local** single-particle (Kohn-Sham) potential $v_{\mathrm{KS}}(\mathbf{r})$, such that the exact ground-state density of the interacting system can be reproduced by non-interacting particles moving in this local potential:

$$\rho(\mathbf{r}) = \rho_{\mathrm{KS}}(\mathbf{r}) \equiv \sum_i^{\mathrm{occ}} |\phi_i(\mathbf{r})|^2$$

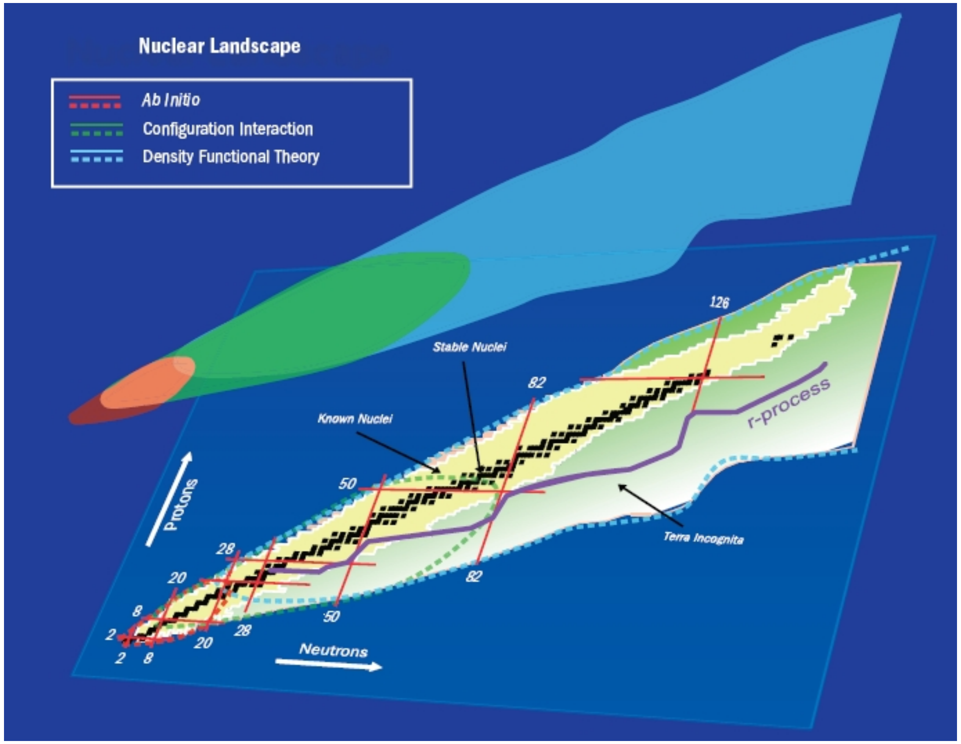
  - ⋆ system energy density functional:

$$E[\rho(\mathbf{r})] = T[\rho(\mathbf{r})] + E_{\mathrm{ext.}}[\rho(\mathbf{r})] + E_{\mathrm{H}}[\rho(\mathbf{r})] + E_{\mathrm{xc}}[\rho(\mathbf{r})]$$

Nuclear DFT

- Nuclear DFT is a promising tool for investigating the ground-state and excited state properties of nuclei throughout the nuclear chart.
- Since the 1970s, lots of experience have been accumulated in implementing, adjusting, and using the DFT in nuclei.

  Petkov&Stoitsov:1991, Bender:2003, Nakatsukasa:2015, ...



http://www.unedf.org/

Covariant density functional theory – RH theory

- The covariant version of DFT takes into account Lorentz symmetry.
  - ⋆ stringent restrictions on the number of parameters

- CDFT in Hartree level (RH/RMF theory) has received wide attention due to its successful description of lots of nuclear phenomena.

  Serot:1986, Ring:1996, Vretenar:2005, Meng:2006, Paar:2007, Nikšić:2011; Meng & Zhou, *JPG* **42**, 093101 (2015)

  - ⋆ spin-orbit splittings, pseudospin symmetry HZL, Meng, Zhou, *Phys. Rep.* **570**, 1–84 (2015)
  - ⋆ EoS in symmetric and asymmetric nuclear matter
  - ⋆ ground-state properties of finite spherical and deformed nuclei
  - ⋆ collective rotational and vibrational excitations
  - ⋆ low-lying spectra of transitional nuclei involving quantum phase transitions
  - ⋆ ......

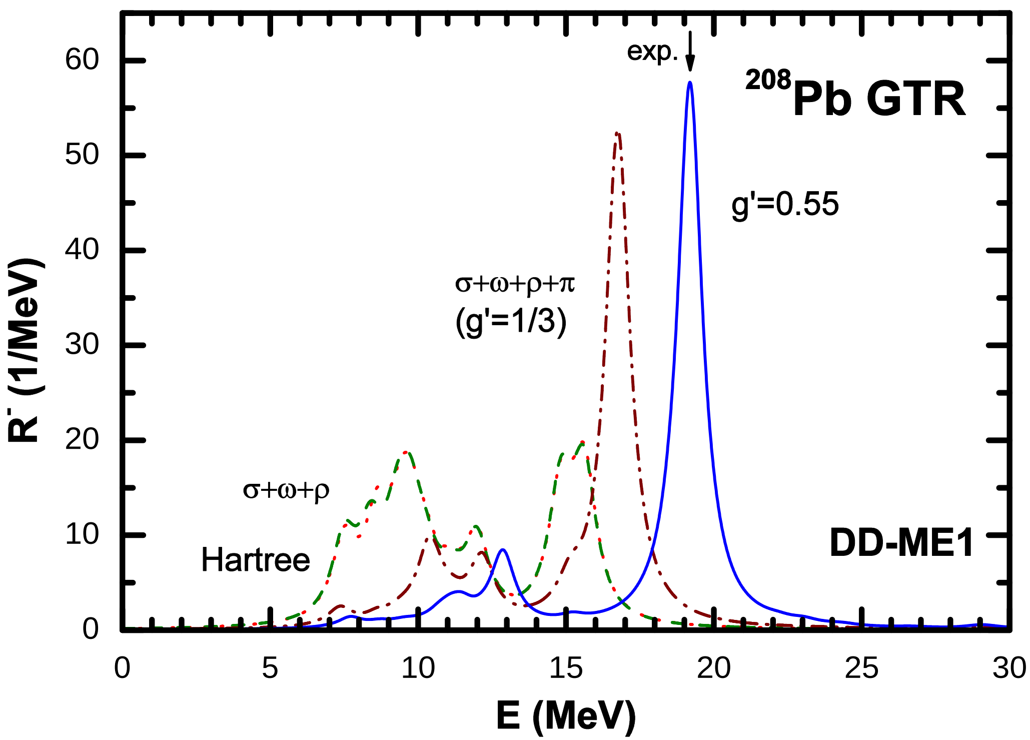
Something more: the isovector channels

- Difficult to disentangle the isovector-scalar (δ) and isovector-vector (ρ) channels, unless a tuning is performed based on selected microscopic calculations. Roca-Maza:2011
- Nuclear spin-isospin resonances, e.g., GTR and SDR, cannot be described in a fully self-consistent way.

RH+RPA for spin-isospin resonances

- RH+RPA for spin-isospin resonances
  De Conti:1998, 2000, Vretenar: 2003, Ma:2004, Paar:2004, Nikšić:2005

example: Gamow-Teller resonance (GTR) in ^{208}Pb ($\Delta S = 1$, $\Delta L = 0$, $J^\pi = 1^+$)



a. add π-meson b. fit g' full self-consistency is missing

Covariant density functional theory – RHF theory

- CDFT in Hartree-Fock level (RHF theory)
  - ⋆ several attempts to include the Fock term in the relativistic framework

    Bouyssy:1985,1987, Bernardos:1993, Marcos:2004
  - ⋆ DDRHF theory achieved quantitative descriptions of binding energies and radii

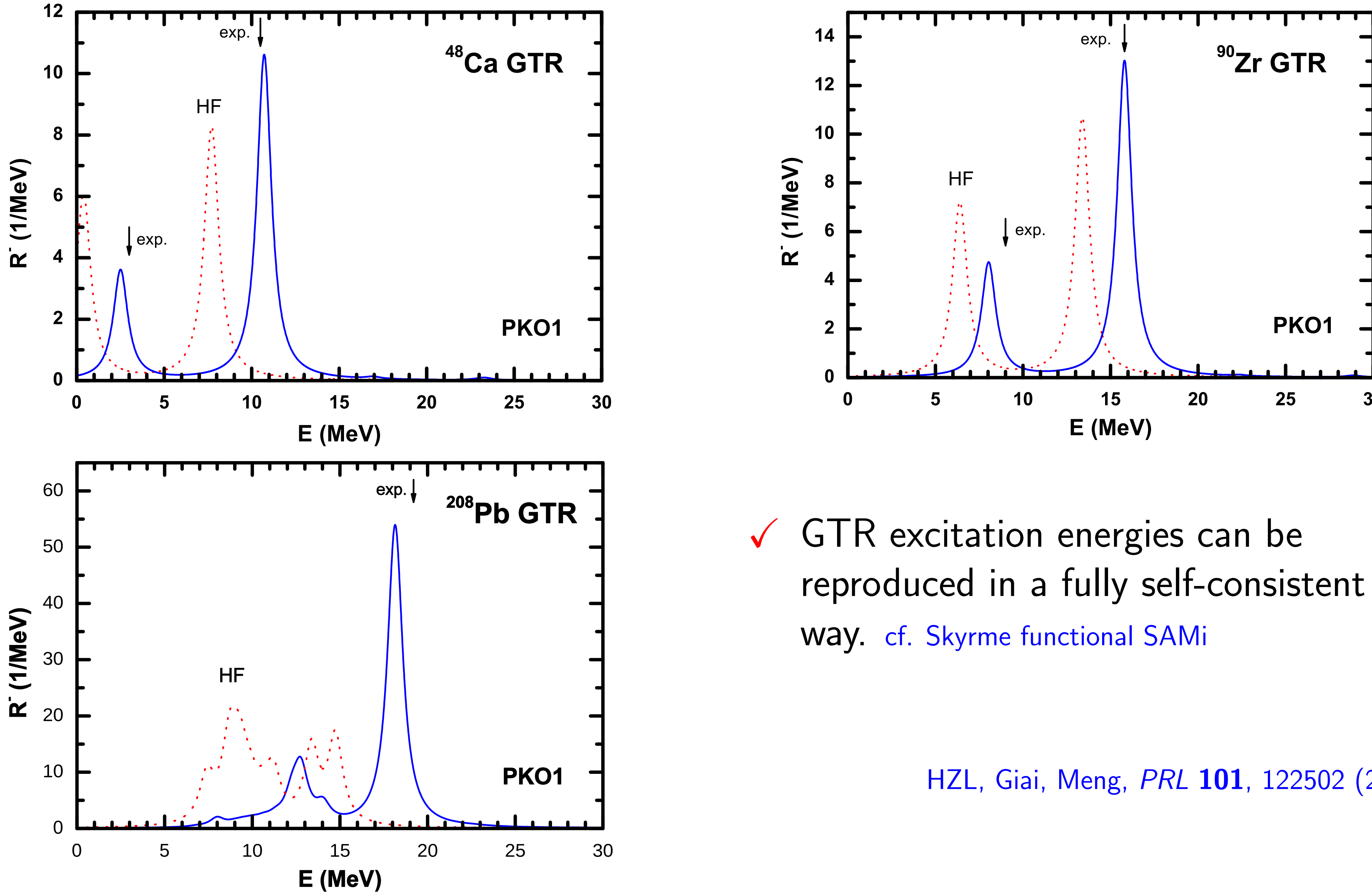
    Long, Giai, Meng, *PLB* **640**, 150 (2006); Long, Sagawa, Giai, Meng, *PRC* **76**, 034314 (2007);
    Long, Sagawa, Meng, Giai, *EPL* **82**, 12001 (2008); Long, Ring, Giai, Meng, *PRC* **81**, 024308 (2010)
  - ⋆ effective mass splitting in asymmetric nuclear matter can be described naturally

    Long, Giai, Meng, *PLB* **640**, 150 (2006)
  - ⋆ nuclear spin-isospin resonances can be described in a fully self-consistent way

    HZL, Giai, Meng, *PRL* **101**, 122502 (2008); HZL, Giai, Meng, *PRC* **79**, 064316 (2009);
    HZL, Zhao, Meng, *PRC* **85**, 064302 (2012)

RHF+RPA for Gamow-Teller resonances

★ Gamow-Teller resonances in ^{48}Ca, ^{90}Zr, and ^{208}Pb



✓ GTR excitation energies can be reproduced in a fully self-consistent way. cf. Skyrme functional SAMi

HZL, Giai, Meng, *PRL* **101**, 122502 (2008)

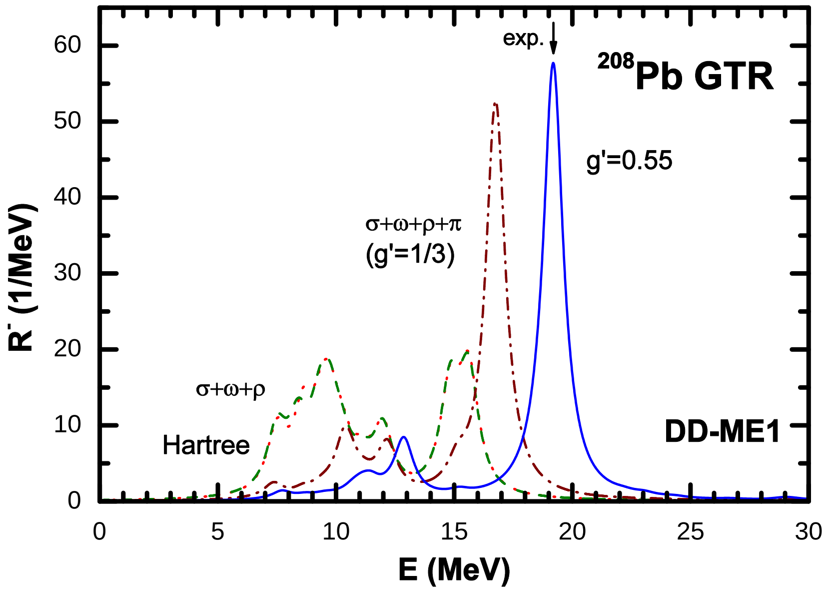
GTR excitation energies and strength

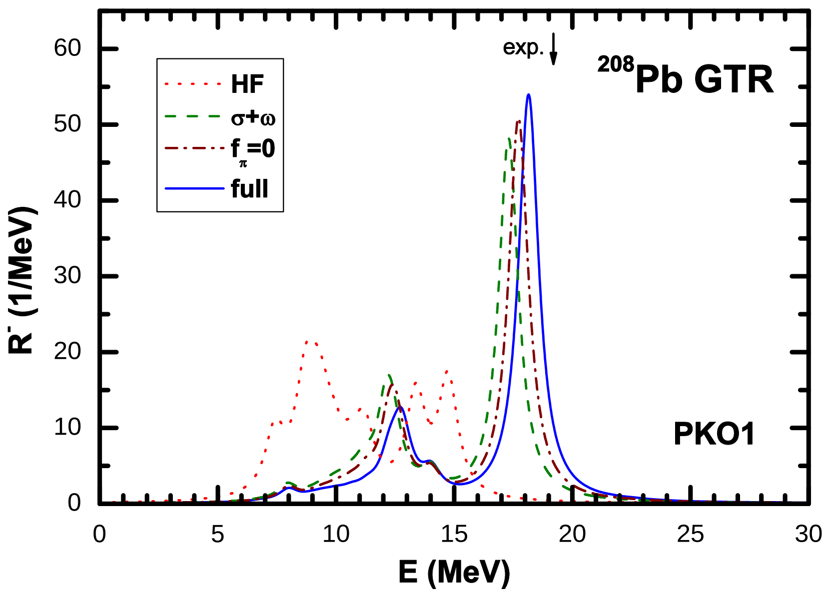
★ GTR excitation energies in MeV and strength in percentage of the $3(N-Z)$ sum rule within the RHF+RPA framework. Experimental and the RH+RPA results are given for comparison.
HZL, Giai, Meng, *PRL* **101**, 122502 (2008)

		^{48}Ca		^{90}Zr		^{208}Pb	
		energy	strength	energy	strength	energy	strength
experiment		~ 10.5		15.6 ± 0.3		19.2 ± 0.2	60-70
RHF+RPA	PKO1	10.72	69.4	15.80	68.1	18.15	65.6
	PKO2	10.83	66.7	15.99	66.3	18.20	60.5
	PKO3	10.42	70.7	15.71	68.9	18.14	67.7
RH+RPA	DD-ME1	10.28	72.5	15.81	71.0	19.19	70.6

- The pion is not included in PKO2.

Physical mechanisms of GTR





- RH+RPA
  - ⋆ no contribution from isoscalar mesons (σ, ω), because exchange terms are missing.
  - ⋆ π-meson is dominant in this resonance.
  - ⋆ g' has to be refitted to reproduce the experimental data.
- RHF+RPA
  - ⋆ isoscalar mesons (σ, ω) play an essential role via the exchange terms.
  - ⋆ π-meson plays a minor role.
  - ⋆ $g' = 1/3$ is kept for self-consistency.

HZL, Giai, Meng, *PRL* **101**, 122502 (2008)

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  - ⋆ nuclear spin-isospin resonances can be described in a fully self-consistent way

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- RHF includes **non-local** potentials $v_{\rm HF}(\mathbf{r}, \mathbf{r}')$, the simplicity of KS scheme is lost.
- RHF is much more complicated than RH theory.
- The computational cost is too expensive for including paring, deformation, projection, cranking, ...

To construct RH functionals from RHF scheme

It is therefore highly desirable

- to stay within the conventional Kohn-Sham scheme in nuclear physics
- to find a covariant density functional based on only local potentials, yet keeping the merits of the exchange terms

- Possible/promising solution: construct RH functionals from RHF scheme
  - ⋆ take the constraints introduced by exchange terms of RHF scheme into account

- We start from an important observation: RHF functional PKO2 [Long:2008]
  - ⋆ well describes the neutron-proton Dirac mass splitting in asymmetric nuclear matter and nuclear spin-isospin resonances
  - ⋆ only includes σ-, ω-, ρ-mesons, but not π-meson
  - ⋆ masses of mesons are heavy $\Rightarrow$ zero-range approximation is reasonable
  - ⋆ Fierz transformation: Fock terms $\Rightarrow$ local Hartree terms

In this work

- To construct RH functional from RHF scheme by the following procedure
  - ⋆ start with RHF parametrization PKO2
  - ⋆ perform the zero-range reduction
  - ⋆ perform the Fierz transformation
- With such RH functional thus obtained, to investigate
  - ⋆ proton-neutron Dirac mass splitting in neutron matter
  - ⋆ Gamow-Teller and spin-dipole resonances

Goal(s)

- To verify whether the important effects of exchange terms can be maintained by the mapping from RHF functional to RH functional.

Covariant density functional theory – RHF theory

- Effective Lagrangian density Bouyssy:1987, Long:2006

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

- System Hamiltonian

$$\mathcal{H} = \mathcal{T}^{00} = \frac{\partial\mathcal{L}}{\partial\dot{\phi}_i}\dot{\phi}_i - \mathcal{L} \quad (2)$$

- Ground-state trial wave function

$$|\Phi_0\rangle = \prod_a c_a^\dagger|0\rangle \quad (3)$$

- Energy functional of the system

$$E = \langle\Phi_0|H|\Phi_0\rangle = E_k + E_\sigma^D + E_\omega^D + E_\rho^D + E_A^D + E_\sigma^E + E_\omega^E + E_\rho^E + E_A^E \quad (4)$$

Zero-range reduction

- Yukawa propagators of the mesons

$$D_i(\mathbf{r},\mathbf{r}') = \frac{1}{4\pi}\frac{e^{-m_i|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}, \qquad D_i(\mathbf{q}) = \frac{1}{m_i^2+\mathbf{q}^2} \tag{5}$$

for $m_i \gg q$,

$$D_i(\mathbf{q}) \approx \frac{1}{m_i^2} - \frac{\mathbf{q}^2}{m_i^4} + \cdots \quad \Rightarrow \quad D_i(\mathbf{r},\mathbf{r}') \approx \frac{1}{m_i^2}\delta(\mathbf{r}-\mathbf{r}') \tag{6}$$

within the zero-order approximation.

- Zero-range reduction of meson-nucleon couplings

$$\alpha_S^{\mathrm{HF}} = -\frac{g_\sigma^2}{m_\sigma^2}, \qquad \alpha_V^{\mathrm{HF}} = \frac{g_\omega^2}{m_\omega^2}, \qquad \alpha_{tV}^{\mathrm{HF}} = \frac{g_\rho^2}{m_\rho^2}, \tag{7}$$

Fierz transformation (I)

- Sixteen Dirac matrices form a complete system

$$O^S = 1, O^V = \gamma^\mu, O^T = \sigma^{\mu\nu}, O^{PS} = \gamma^5, O^{PV} = \gamma^5\gamma^\mu$$

so that any one can be expressed as a linear superposition of variants with a changed sequence of spinors,

$$(\bar{a}O^i d)(\bar{c}O_i b) = \sum_k c_{ik}(\bar{a}O^k b)(\bar{c}O_k d), \tag{8}$$

with the coefficients c_{ik} in the so-called Fierz table Fierz:1937, Okun:1982, Sulaksono:2003

$$\begin{array}{cccccc} & S & V & T & PS & PV \\ S & \frac{1}{4} & \frac{1}{4} & \frac{1}{8} & \frac{1}{4} & -\frac{1}{4} \\ V & 1 & -\frac{1}{2} & 0 & -1 & -\frac{1}{2} \\ T & 3 & 0 & -\frac{1}{2} & 3 & 0 \\ PS & \frac{1}{4} & -\frac{1}{4} & \frac{1}{8} & \frac{1}{4} & \frac{1}{4} \\ PV & -1 & -\frac{1}{2} & 0 & 1 & -\frac{1}{2} \end{array} \tag{9}$$

- For the isospin coefficients,

$$\delta_{q_a q_d}\delta_{q_c q_b} = \frac{1}{2}\left[\delta_{q_a q_b}\delta_{q_c q_d} + \langle q_a|\vec{\tau}|q_b\rangle \cdot \langle q_c|\vec{\tau}|q_d\rangle\right], \tag{10a}$$

$$\langle q_a|\vec{\tau}|q_d\rangle \cdot \langle q_c|\vec{\tau}|q_b\rangle = \frac{1}{2}\left[3\delta_{q_a q_b}\delta_{q_c q_d} - \langle q_a|\vec{\tau}|q_b\rangle \cdot \langle q_c|\vec{\tau}|q_d\rangle\right]. \tag{10b}$$

Fierz transformation (II)

- Fierz transformation: from α^{HF} to α^{H}

$$\alpha_S^{\mathrm{H}} = +\frac{7}{8}\alpha_S^{\mathrm{HF}} - \frac{4}{8}\alpha_V^{\mathrm{HF}} - \frac{12}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11a}$$

$$\alpha_{tS}^{\mathrm{H}} = -\frac{1}{8}\alpha_S^{\mathrm{HF}} - \frac{4}{8}\alpha_V^{\mathrm{HF}} + \frac{4}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11b}$$

$$\alpha_V^{\mathrm{H}} = -\frac{1}{8}\alpha_S^{\mathrm{HF}} + \frac{10}{8}\alpha_V^{\mathrm{HF}} + \frac{6}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11c}$$

$$\alpha_{tV}^{\mathrm{H}} = -\frac{1}{8}\alpha_S^{\mathrm{HF}} + \frac{2}{8}\alpha_V^{\mathrm{HF}} + \frac{6}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11d}$$

$$\alpha_T^{\mathrm{H}} = -\frac{1}{16}\alpha_S^{\mathrm{HF}} \tag{11e}$$

$$\alpha_{tT}^{\mathrm{H}} = -\frac{1}{16}\alpha_S^{\mathrm{HF}} \tag{11f}$$

$$\alpha_{PS}^{\mathrm{H}} = -\frac{1}{8}\alpha_S^{\mathrm{HF}} + \frac{4}{8}\alpha_V^{\mathrm{HF}} + \frac{12}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11g}$$

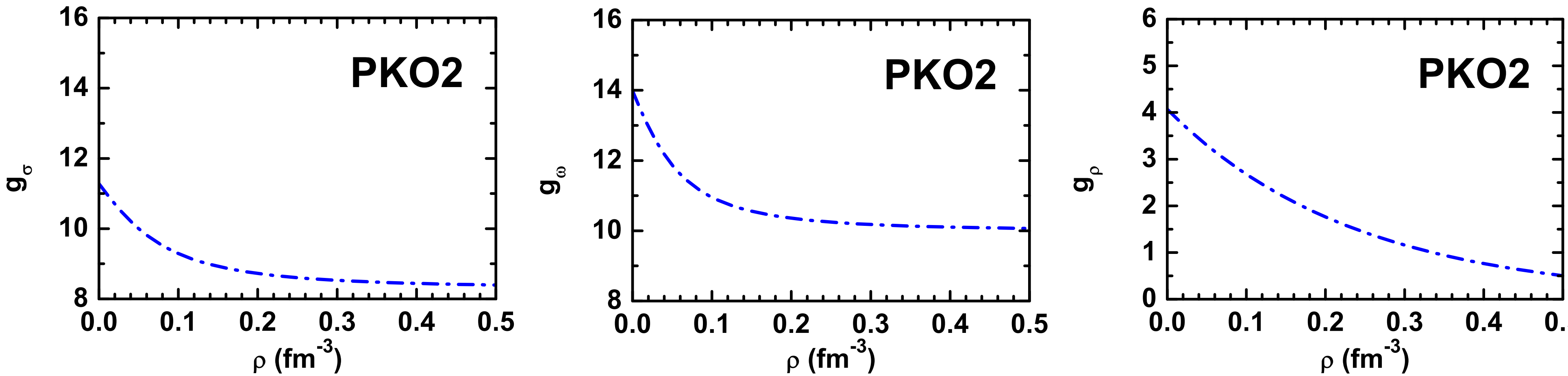
$$\alpha_{tPS}^{\mathrm{H}} = -\frac{1}{8}\alpha_S^{\mathrm{HF}} + \frac{4}{8}\alpha_V^{\mathrm{HF}} - \frac{4}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11h}$$

$$\alpha_{PV}^{\mathrm{H}} = +\frac{1}{8}\alpha_S^{\mathrm{HF}} + \frac{2}{8}\alpha_V^{\mathrm{HF}} + \frac{6}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11i}$$

$$\alpha_{tPV}^{\mathrm{H}} = +\frac{1}{8}\alpha_S^{\mathrm{HF}} + \frac{2}{8}\alpha_V^{\mathrm{HF}} - \frac{2}{8}\alpha_{tV}^{\mathrm{HF}} \tag{11j}$$

Nucleon-meson coupling strengths of PKO2

- Starting point: nucleon-meson coupling strengths g_σ, g_ω, and g_ρ of PKO2



Long, Sagawa, Meng, Giai, *EPL* **82**, 12001 (2008)

- Zero-range reduction

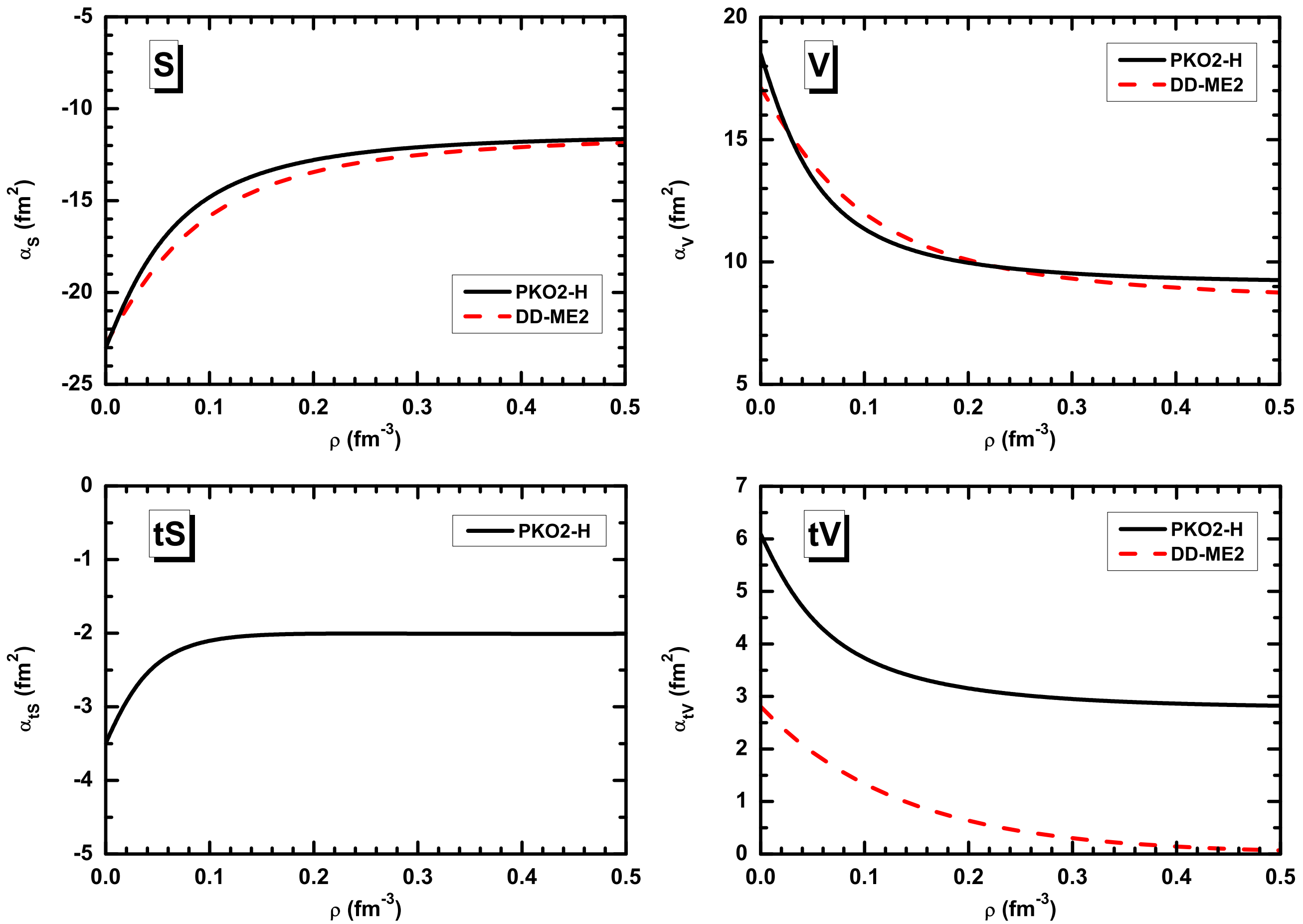
$$\alpha_S^{\rm HF} = -\frac{g_\sigma^2}{m_\sigma^2}, \qquad \alpha_V^{\rm HF} = \frac{g_\omega^2}{m_\omega^2}, \qquad \alpha_{tV}^{\rm HF} = \frac{g_\rho^2}{m_\rho^2},$$

- Fierz transformation

$$\alpha_j^{\rm H} = \sum_k c_{jk}\alpha_k^{\rm HF},$$

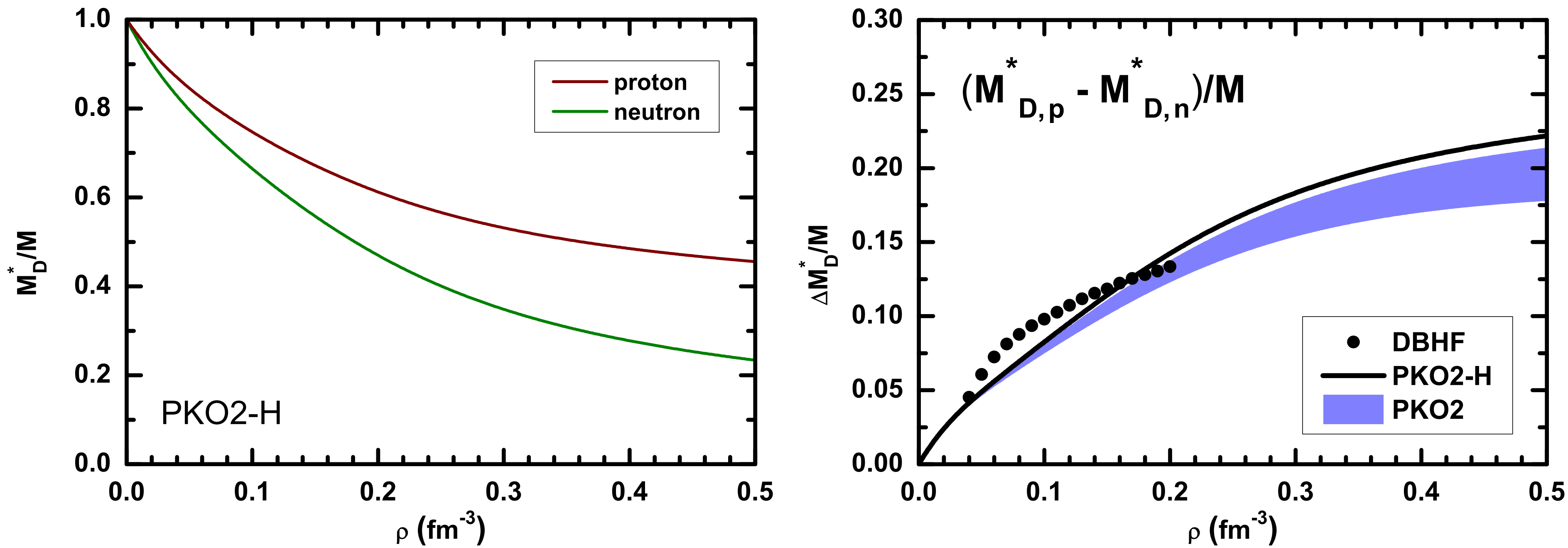
RHF equivalent zero-range coupling strengths (I)

- The RHF equivalent parametrization derived from PKO2 is called "**PKO2-H**".



- α_S^{H} and α_V^{H} are consistent with those of DD-ME2 Lalazissis:2005
- α_{tS}^{H} appears $\Rightarrow$ proton-neutron Dirac mass splitting in asymmetric nuclear matter
- α_{tV}^{H} is modified for another delicate balance between tS and tV channels

Dirac mass and its isospin splitting

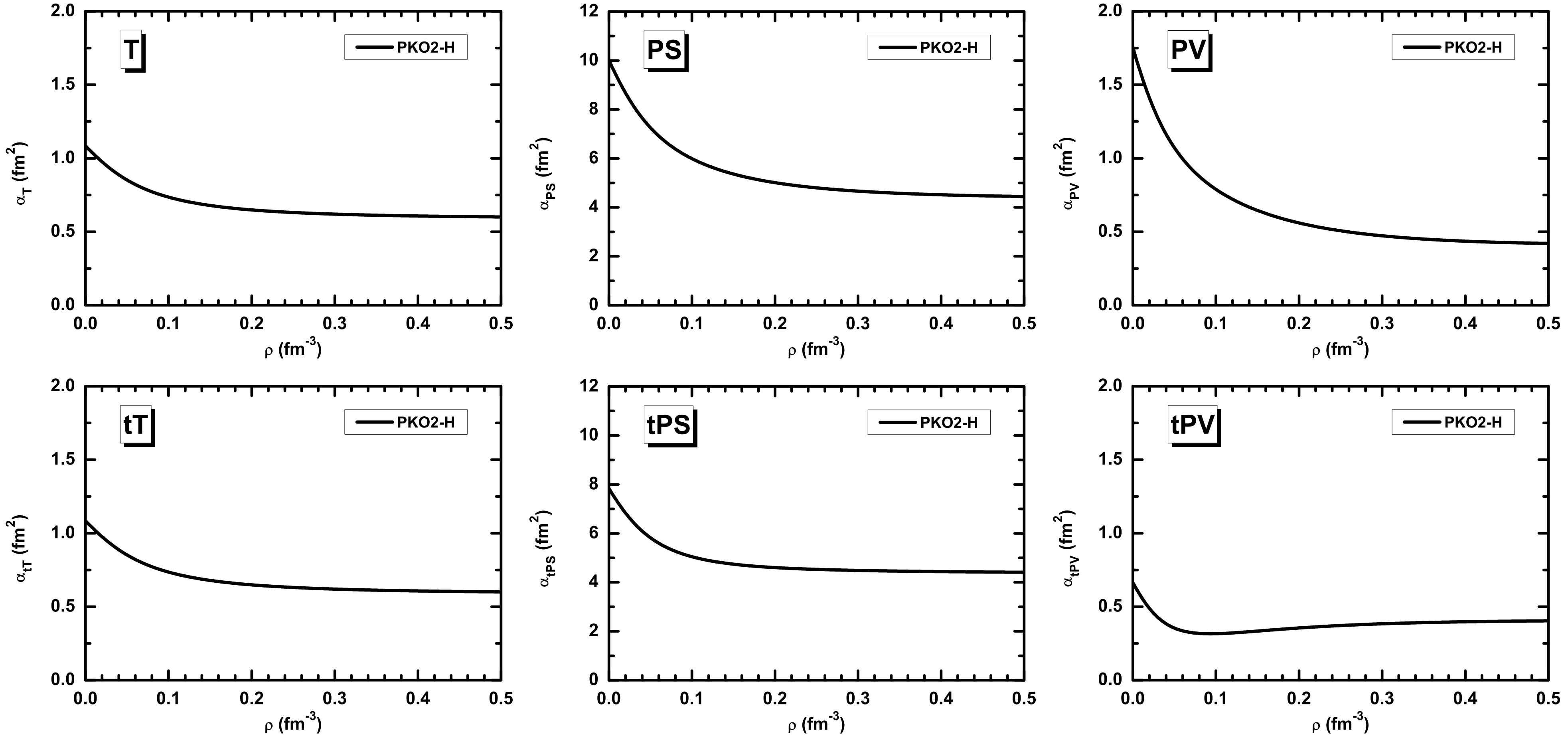


DBHF: van Dalen, *et al.*, *EPJA* **31**, 29 (2007)

- It is found that $M^*_{D,p} > M^*_{D,n}$.
- The splitting behavior in neutron matter is quantitatively consistent with the prediction of the Dirac-Brueckner-Hartree-Fock (DBHF) calculations.

- The constraints introduced by the Fock terms of the RHF scheme into the *tS* channel of the present density functional are straight forward and quite robust.

RHF equivalent zero-range coupling strengths (II)



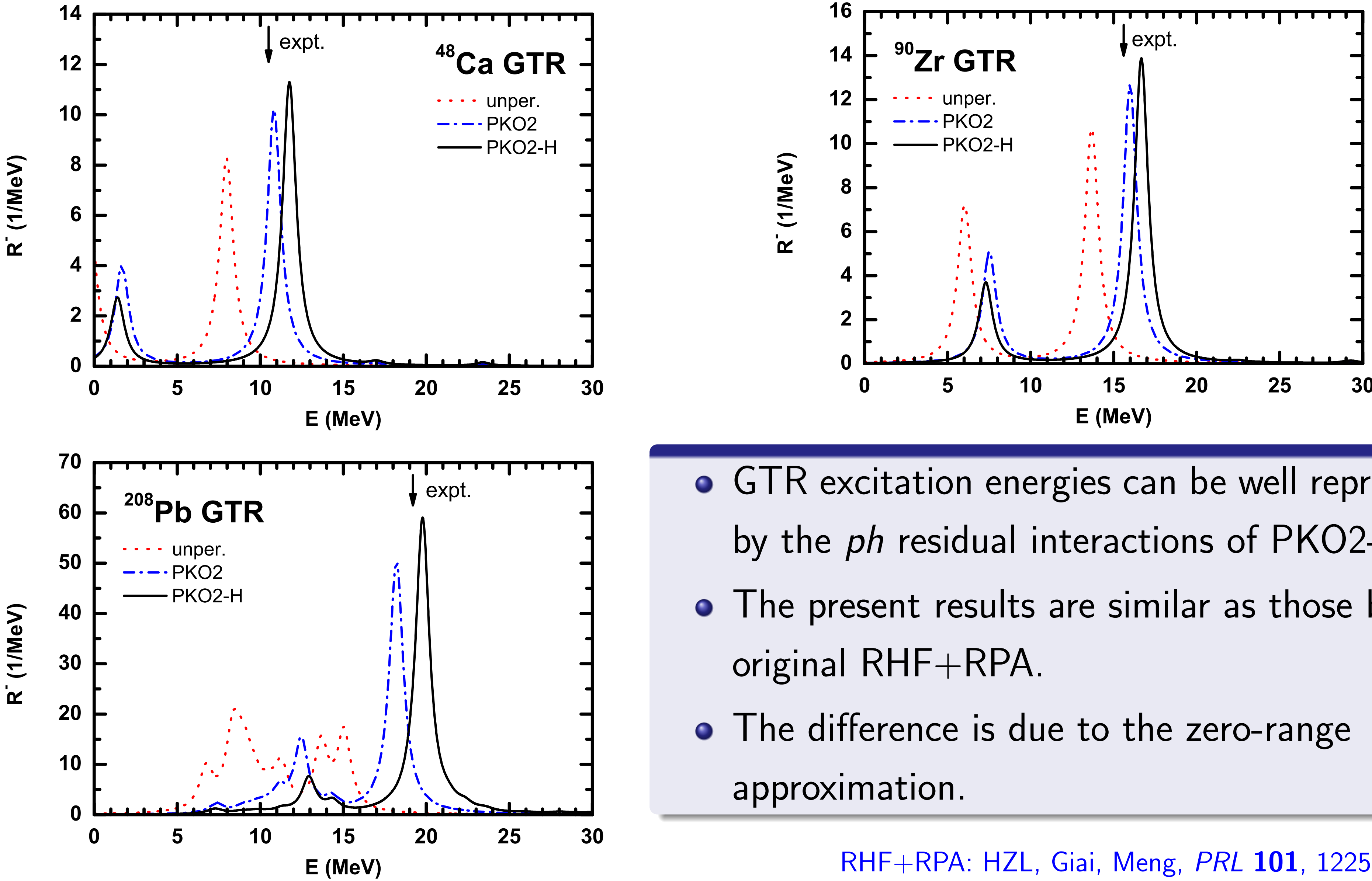
- $\alpha^{\mathrm{H}}_{(t)T}$, $\alpha^{\mathrm{H}}_{(t)PS}$, and $\alpha^{\mathrm{H}}_{(t)PV}$ are explicitly determined by exchange effects of RHF scheme
- $(t)PS$ and $(t)PV$ channels vanish in ground-state descriptions due to the parity conservation, but crucial for spin-isospin resonances

Particle-hole residual interactions in charge-exchange channel

- Particle-hole (ph) residual interactions
  - tS channel: $$V_{tS}(1,2) = \alpha^{\rm H}_{tS}[\gamma_0\vec{\tau}]_1 \cdot [\gamma_0\vec{\tau}]_2\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{12a}$$
  - tV channel: $$V_{tV}(1,2) = \alpha^{\rm H}_{tV}[\gamma_0\gamma^\mu\vec{\tau}]_1 \cdot [\gamma_0\gamma_\mu\vec{\tau}]_2\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{12b}$$
  - tT channel: $$V_{tT}(1,2) = \alpha^{\rm H}_{tT}[\gamma_0\sigma^{\mu\nu}\vec{\tau}]_1 \cdot [\gamma_0\sigma_{\mu\nu}\vec{\tau}]_2\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{12c}$$
  - tPS channel: $$V_{tPS}(1,2) = \alpha^{\rm H}_{tPS}[\gamma_0\gamma_5\vec{\tau}]_1 \cdot [\gamma_0\gamma_5\vec{\tau}]_2\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{12d}$$
  - tPV channel: $$V_{tPV}(1,2) = \alpha^{\rm H}_{tPV}[\gamma_0\gamma_5\gamma^\mu\vec{\tau}]_1 \cdot [\gamma_0\gamma_5\gamma_\mu\vec{\tau}]_2\delta(\mathbf{r}_1 - \mathbf{r}_2). \tag{12e}$$

- For the charge-exchange spin-flip modes, the tT and tPV channels are expected to play the dominant roles, where the operator $[\boldsymbol{\sigma}\vec{\tau}] \cdot [\boldsymbol{\sigma}\vec{\tau}]$ is sandwiched by the large components of wave functions.

Gamow-Teller resonances

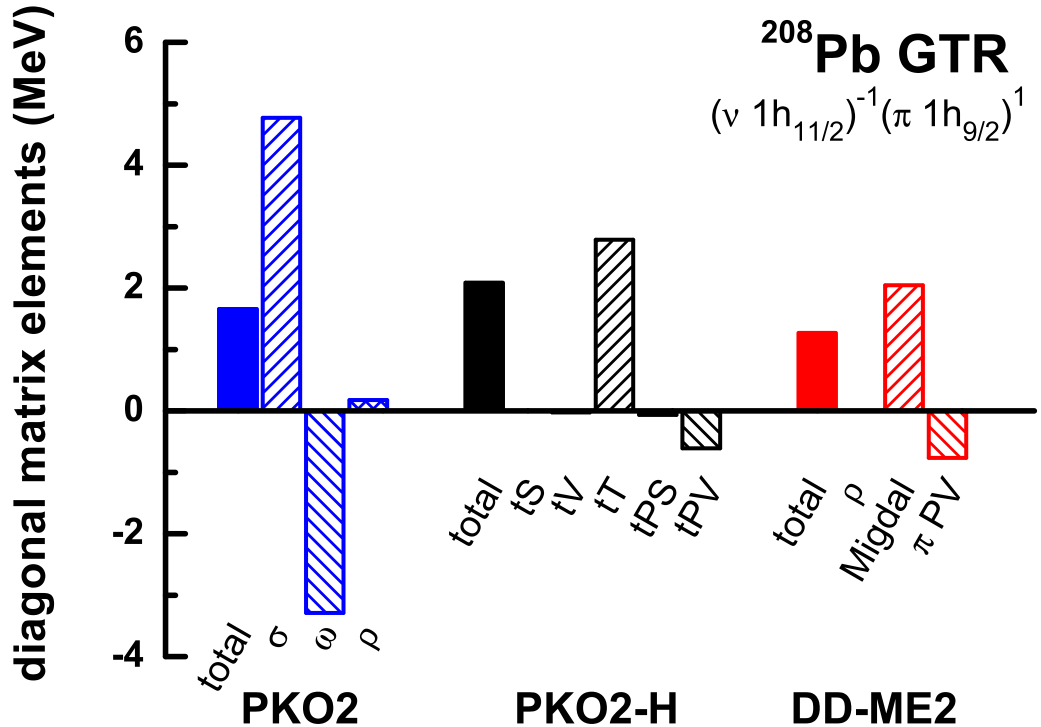


- GTR excitation energies can be well reproduced by the *ph* residual interactions of PKO2-H.
- The present results are similar as those by the original RHF+RPA.
- The difference is due to the zero-range approximation.

RHF+RPA: HZL, Giai, Meng, *PRL* **101**, 122502 (2008)

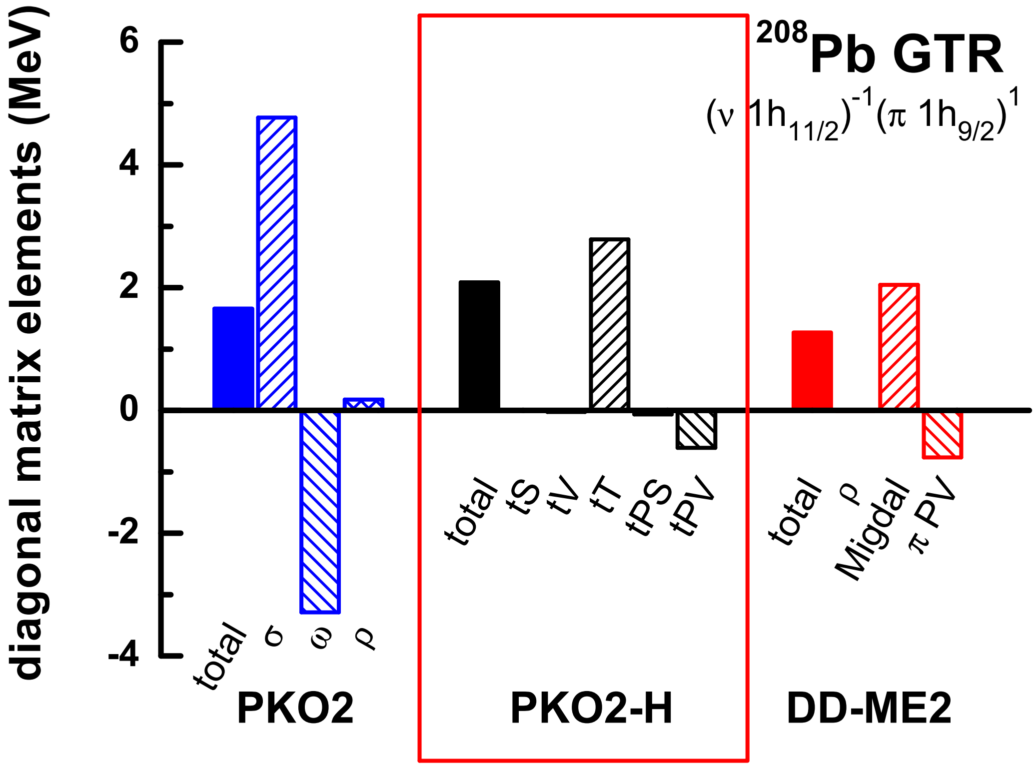
localized RHF+RPA: HZL, Zhao, Ring, Roca-Maza, Meng, *PRC* **86**, 021302(R) (2012)

Physical mechanisms of GTR



- In RHF+RPA (PKO2), σ- and ω-mesons play the most important role in determining the properties of GTR via the exchange terms.
- In the RHF equivalent RPA (PKO2-H), tT and tPV channels are most important, their coupling strengths are intrinsically determined by Fierz transformation.
- In conventional RH+RPA (DD-ME2), the free π residual interaction is attractive and the Migdal term is repulsive by fitting to experimental data.

Physical mechanisms of GTR by PKO2-H

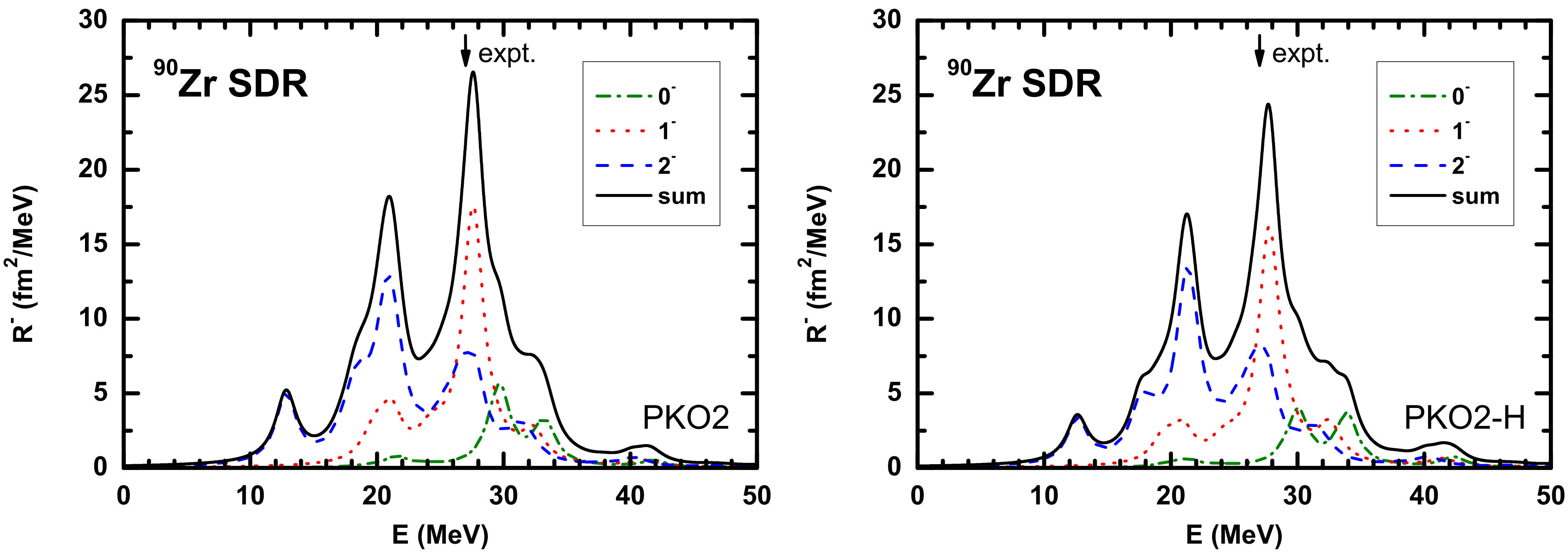


- The dominant *ph* interactions are the operator $[\boldsymbol{\sigma}\vec{\tau}] \cdot [\boldsymbol{\sigma}\vec{\tau}]$ sandwiched by large components of w.f., i.e., $[\sigma^{ij}\vec{\tau}] \cdot [\sigma_{ij}\vec{\tau}] \propto 2\alpha_{tT}^{\mathrm{H}}$ and $[\gamma_5\gamma^i\vec{\tau}] \cdot [\gamma_5\gamma_i\vec{\tau}] \propto -\alpha_{tPV}^{\mathrm{H}}$
- The net contribution is then proportional to

$$2\alpha_{tT}^{\mathrm{H}} - \alpha_{tPV}^{\mathrm{H}} = -\frac{1}{3}\left(\alpha_S^{\mathrm{H}} + \alpha_V^{\mathrm{H}}\right)$$

- Total *ph* strengths are determined by the delicate balance between S and V channels.

Spin-dipole resonances

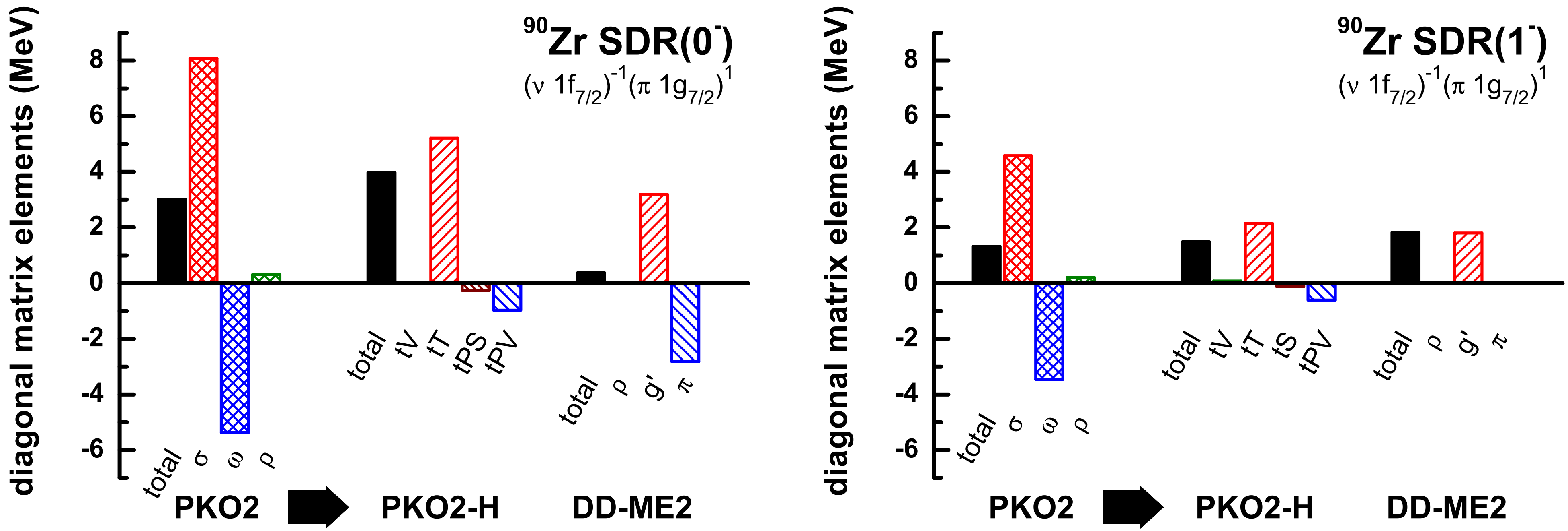


expt: Yako, Sagawa, Sakai, *PRC* **74**, 051303 (2006)

- Not only the total strengths but also the individual contribution from different spin-parity J^{π} components are almost identical.
- The energy hierarchy $E(2^-) < E(1^-) < E(0^-)$ can be obtained naturally in the present RPA calculations in the local scheme.

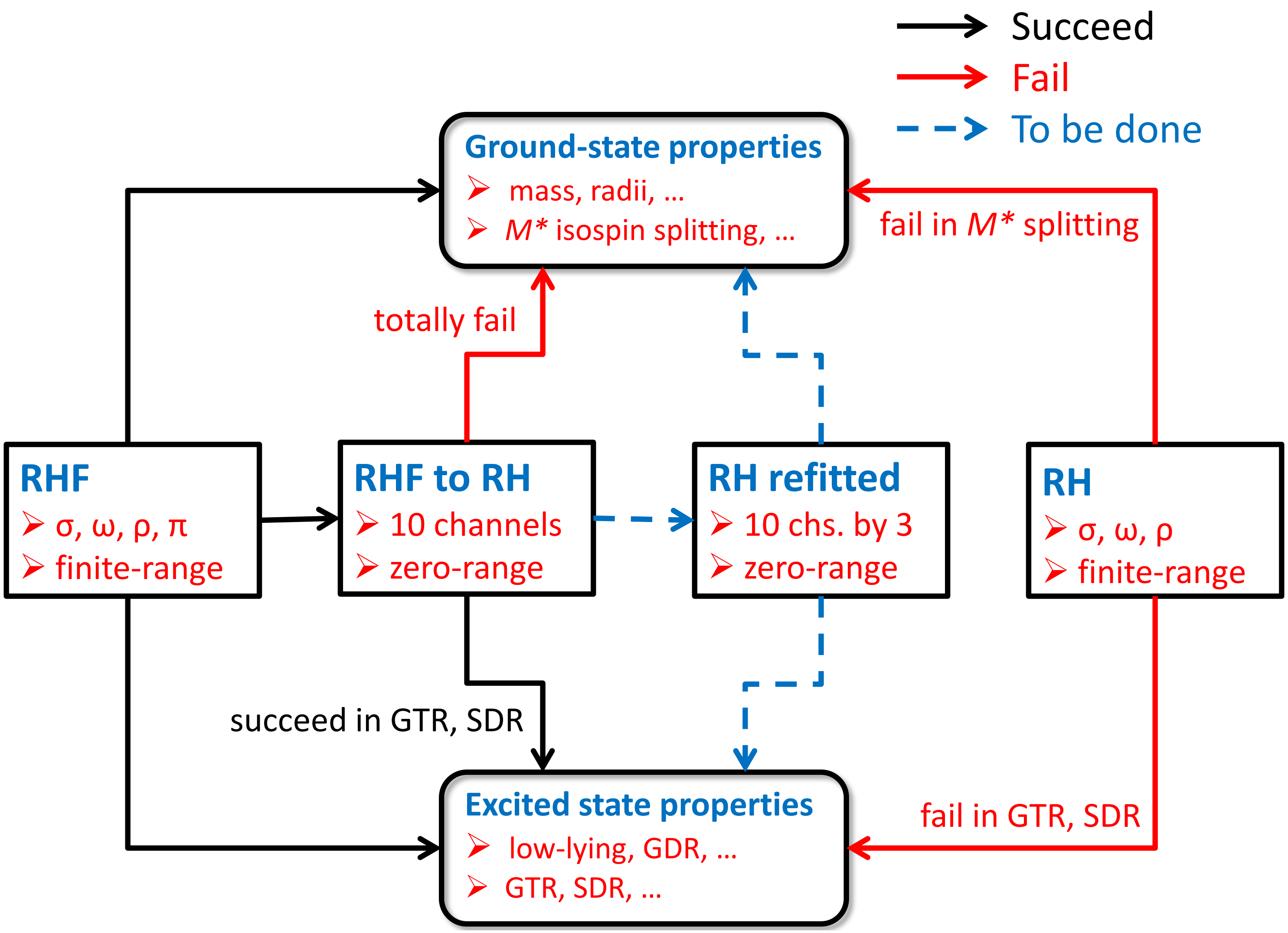
- The constraints introduced by the Fock terms of the RHF scheme into the *ph* residual interactions are also straight forward and quite robust.

Physical mechanisms of SDR



- In RHF+RPA, the balance between σ- and ω-mesons are most important.
- In the Hartree equivalent RPA, the tT and tPV channels are most important.
- In conventional RH+RPA, the balance between the free π and g' terms are changed in different J^π components, this leads to $E(0^-) < E(1^-)$.

Strategy map



⋆ Zhaoxi Li (Beihang) → RIKEN IPA project (2015.10 – 2016.3)

Summary and Perspectives

Summary

★ A new method is proposed to take into account the Fock terms in local covariant density functionals.

✓ The advantages of existing RH functionals can be maintained, while the problems in the isovector channel can be solved.

- ⋆ The neutron-proton Dirac mass splitting in asymmetric nuclear matter is in a very good agreement with the prediction of DBHF.
- ⋆ The properties of GTR and SDR can be reproduced in a natural way.

Perspectives

- This opens a new door for the development of nuclear local covariant density functionals with proper isoscalar and isovector properties in the future.

Thank you!