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Skyrme functional with tensor terms from ab initio calculations of neutron-proton drops

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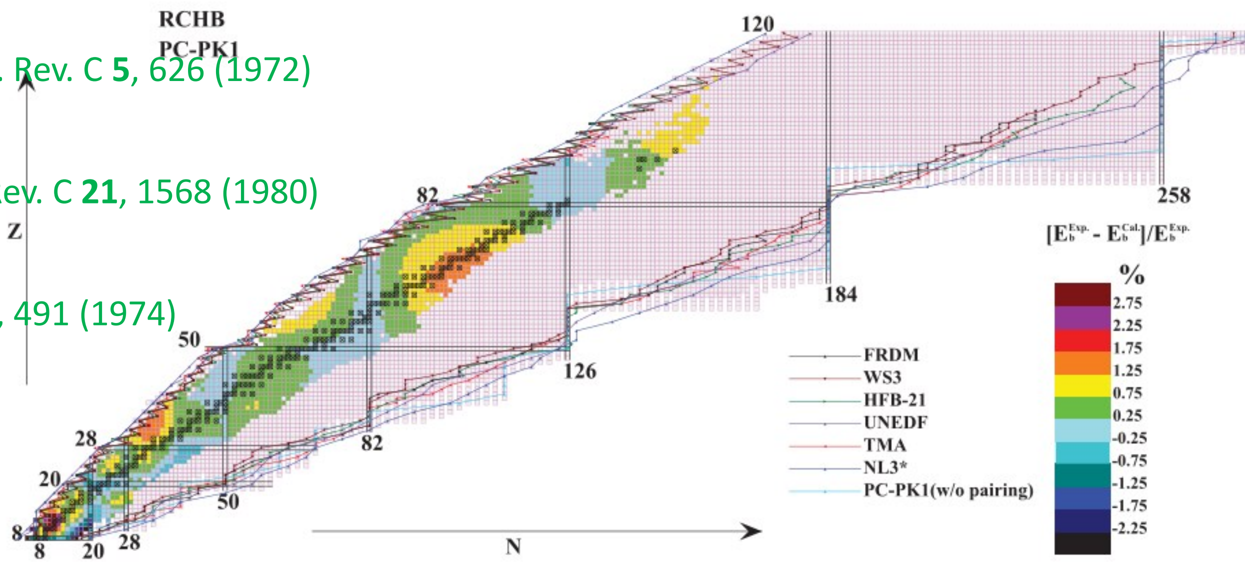
Collaborators: Gianluca Colò and Xavier Roca-Maza

Nuclear Energy Density Functional

- Nuclear energy density functional (EDF) is an important tool in nuclear physics
  M. Bender and P.-h. Heenen, Rev. Mod. Phys. **75**, 121 (2003)
  - Skyrme
    D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972)
  - Gogny
    J. Decharg´ e and D. Gogny, Phys. Rev. C **21**, 1568 (1980)
  - Relativistic
    J. D. Walecka, Ann. Phys. (N. Y). **83**, 491 (1974)



X.W. Xia et al. At Data Nucl. Data Tables, 2018, 121–122: 1

- Open questions still exist regarding current functionals:
  - Symmetry energy M. Baldo and G. Burgio, Prog. Part. Nucl. Phys. **91**, 203 (2016)
  - Tensor force H. Sagawa and G. Colò, Prog. Part. Nucl. Phys. **76**, 76 (2014)
  - … …

Tensor Force

- Experimental facts for tensor force in nucleon-nucleon (NN) interaction:
  - Quadrupole moment of deuteron
  - Nonvanishing transition amplitude from L = J – 1 to L = J + 1 in NN scattering

R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989)

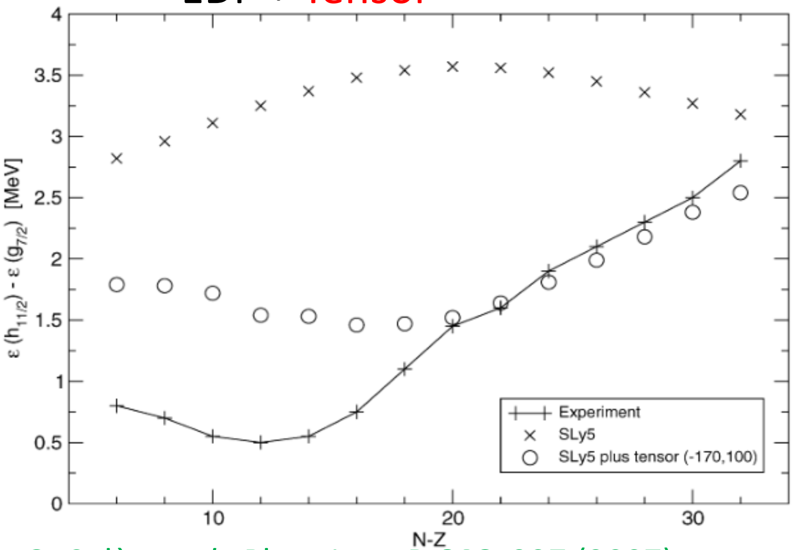
$$V_T = f(r) S_{12},$$

$$S_{12} = 3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

- Tensor force in nuclear medium (EDF): still in debate.

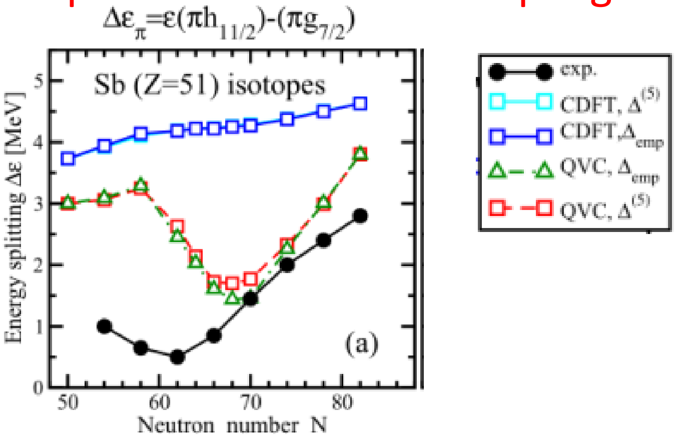
H. Sagawa and G. Colò, *Prog. Part. Nucl. Phys.* **76**, 76 (2014)

EDF + Tensor



G. Colò, *et al*., Phys. Lett. B **646**, 227 (2007)

EDF -> particle-vibrational coupling



A. V. Afanasjev, E. Litvinova, *Phys. Rev. C* **92**, 044317 (2015)

Let ab initio calculation (without PVC) tells us the tensor

Ab initio Calculations

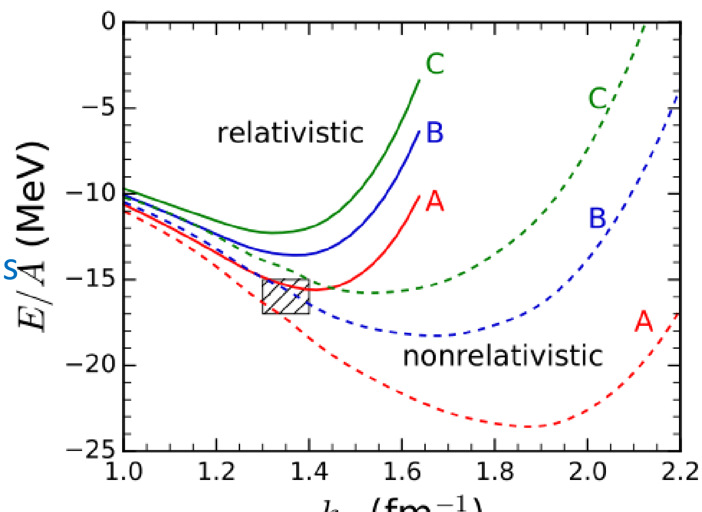
- *ab initio*: describing nucleus from underlying NN interactions

- Brueckner-Hartree-Fock (BHF) theory B. Day, *Rev. Mod. Phys.* **39**, 719 (1967)
- self-consistent Green's function W. Dickhoff and C. Barbieri, Prog. Part. Nucl. Phys. **52**, 377 (2004)
- nuclear lattice effective field theory D. Lee, Prog. Part. Nucl. Phys. **63**, 117 (2009)
- no core shell model B. R. Barrett, P. Navrátil, J. P. Vary, *PPNP* **69**, 131 (2013)
- coupled-cluster theory G. Hagen, et al., *Rep. Prog. Phys.* **77**, 096302 (2014)
- quantum Monte Carlo method J. Carlson, et al., *RMP* **87**, 1067 (2015)
- in medium similarity renormalization group H. Hergert, et al., Phys. Rep. 621, 165 (2016)
- … …

- Relativistic Brueckner-Hartree-Fock (RBHF) theory

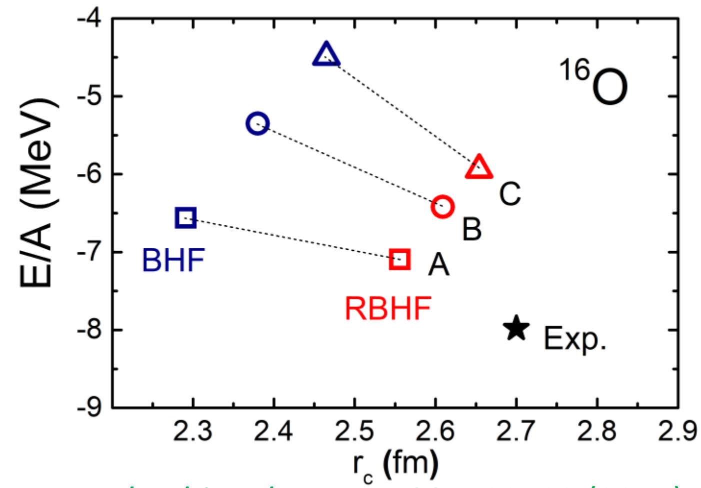
EoS of symmetric nuclear matter by BHF and RBHF with Bonn A, B, C interactions

R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989)



R. Brockmann and R. Machleidt, *PRC* **42**, 1965 (1990)

Energy per nucleon and charge radius of 16O

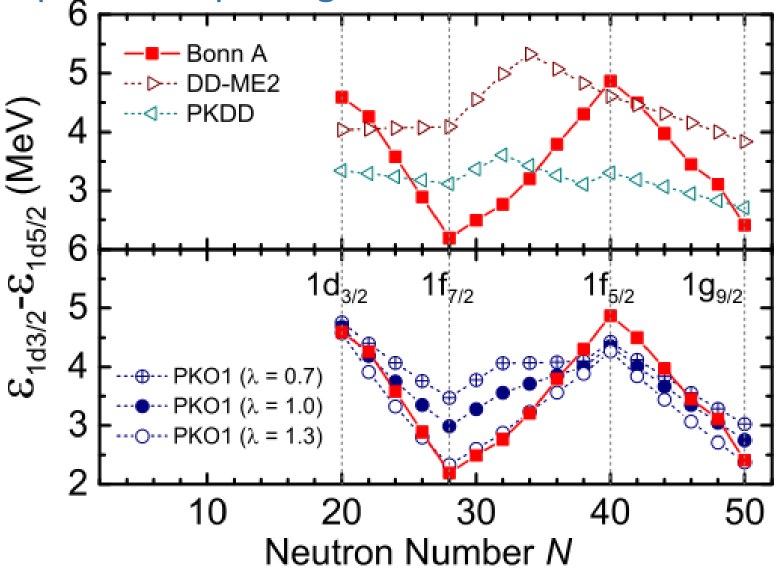


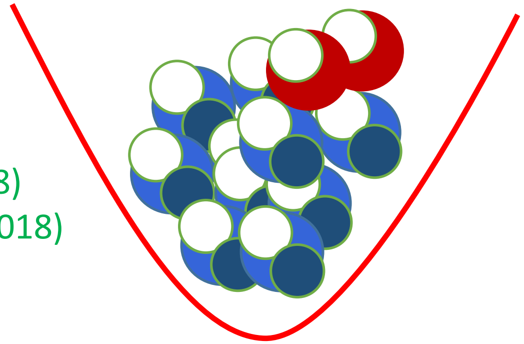
S. Shen, *et al.*, *Chin. Phys. Lett.* **33**, 102103 (2016)
S. Shen, *et al.*, *PRC* **96**, 014316 (2017)

Pseudodata from *ab initio* Calculations

- Relativistic Brueckner-Hartree-Fock theory with Bonn A interaction for neutron drops.

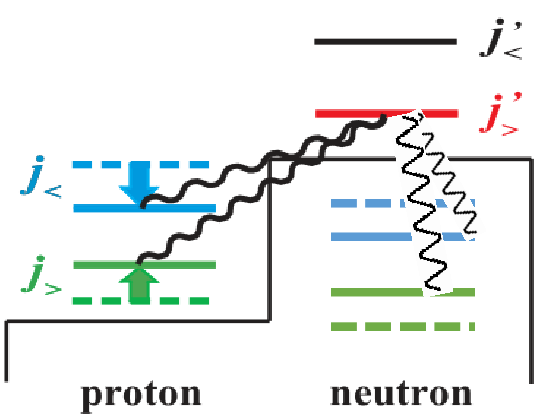
Spin-orbit splitting of 1d orbital as a function of neutron numbers





S. Shen, *et al.*, *PLB* **778**, 344 (2018)
S. Shen, *et al.*, *PRC* **97**, 054312 (2018)

- The SO splitting decreases as the next higher j' = j'> = l' + 1/2 orbit is filled, and recover when next lower j' = j'< = l' – 1/2 is filled.
- Such pattern of SO splitting is not obvious in functionals without tensor force (DD-ME2, PKDD) and can be reproduced by functional with tensor force (PKO1).



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

PRESENT WORK

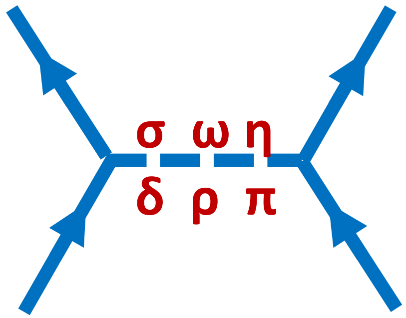
To develop new skyrme functional with tensor force guided by RBHF study in neutron(-proton) drops.

Relativistic Brueckner-Hartree-Fock Theory

- Starting point: Bonn interaction R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989)

  The interaction Lagrangians are defined as

$$
\begin{aligned}
\mathscr{L}_{NNpv} &= -\frac{f_{ps}}{m_{ps}}\bar{\psi}\gamma^5\gamma^\mu\psi\partial_\mu\varphi^{(ps)}, \\
\mathscr{L}_{NNs} &= g_s\bar{\psi}\psi\varphi^{(s)}, \\
\mathscr{L}_{NNv} &= -g_v\bar{\psi}\gamma^\mu\psi\varphi_\mu^{(v)} - \frac{f_v}{4M}\bar{\psi}\sigma^{\mu\nu}\psi\left(\partial_\mu\varphi_\nu^{(v)} - \partial_\nu\varphi_\mu^{(v)}\right) .
\end{aligned}
$$

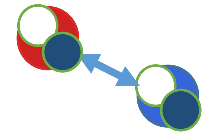


- Bosons to be exchanged include σ, δ (scalar); ω, ρ (vector); η, π (pseudoscalar).
- Coupling constants are determined by NN scattering and deuteron properties R. Machleidt, *Adv. Nucl. Phys.* **19**, 189 (1989).

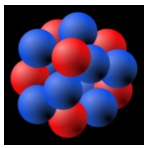
Relativistic Brueckner-Hartree-Fock Theory

K. A. Brueckner, C. A. Levinson, and H. M. Mahmoud, *Phys. Rev.* **95**, 217 (1954)

- Bethe-Goldstone equation



bare interaction in the free space



[redacted]

effective interaction in the nuclear medium

H. A. Bethe and J. Goldsteon, *Proc. R. Soc. A* **238**, 551 (1957)

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

- Q is the Pauli operator which forbids the states being scattered below Fermi surface.

$$Q = \begin{cases} 1, & e_m, e_n > e_F \\ 0, & e_m \leq e_F \text{ or } e_n \leq e_F \end{cases}$$

- W is the so-called starting energy.

Relativistic Brueckner-Hartree-Fock Theory

- Relativistic Hartree-Fock (RHF) equation in complete basis, for details, e.g. W.-H. Long, N. Van Giai, and J. Meng, *PLB* **640**, 150 (2006)

$$\sum_j (T_{ij} + U_{ij}) D_{ja} = \varepsilon_a D_{ia}, \qquad U_{ij} = \sum_{c=1}^{A} \langle ic|\bar{G}(W)|jc\rangle$$

where D are the expansion coefficients: $|a\rangle = \sum_i D_{ia}|i\rangle.$

$$U_{\rm HO}(\mathbf{r}) = \frac{1}{2} M\omega^2 r^2.$$

external field for neutron(-proton) drops

- RBHF total energy

$$E = \sum_a^A \langle a|T|a\rangle + \frac{1}{2}\sum_{ab}^{A} \langle ab|\bar{G}(W)|ab\rangle.$$

for more detail, see S. Shen, *et al.*, *Chin. Phys. Lett.* **33**, 102103 (2016)
S. Shen, *et al.*, *PRC* **96**, 014316 (2017)
S. Shen, *et al.*, *PLB* **781**, 227 (2018)

Skyrme Functional

- Skyrme effective interaction D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972)

$$V(\mathbf{r}_1,\mathbf{r}_2) = t_0(1+x_0P_\sigma)\delta(\mathbf{r}) + \frac{1}{2}t_1(1+x_1P_\sigma)\left[\mathbf{P}'^2\delta(\mathbf{r})+\delta(\mathbf{r})\mathbf{P}^2\right] + t_2(1+x_2P_\sigma)\mathbf{P}'\cdot\delta(\mathbf{r})\mathbf{P},$$
$$+\frac{1}{6}t_3(1+x_3P_\sigma)\rho^\gamma(\mathbf{R})\delta(\mathbf{r}) + iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot[\mathbf{P}'\times\delta(\mathbf{r})\mathbf{P}] + V_T(\mathbf{r}_1,\mathbf{r}_2),$$
$$V_T(\mathbf{r}_1,\mathbf{r}_2) = \frac{T}{2}\left\{\left[(\boldsymbol{\sigma}_1\cdot\mathbf{k}')(\boldsymbol{\sigma}_2\cdot\mathbf{P}') - \frac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\mathbf{P}'^2\right]\delta(\mathbf{r}) + \delta(\mathbf{r})\left[(\boldsymbol{\sigma}_1\cdot\mathbf{P})(\boldsymbol{\sigma}_2\cdot\mathbf{P}) - \frac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\mathbf{P}^2\right]\right\}$$
$$+U\left\{(\boldsymbol{\sigma}_1\cdot\mathbf{P}')\delta(\mathbf{r})(\boldsymbol{\sigma}_2\cdot\mathbf{P}) - \frac{1}{3}(\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\left[\mathbf{P}'\cdot\delta(\mathbf{r})\mathbf{P}\right]\right\},$$

- Hartree-Fock equation

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + U_q(\mathbf{r})\right]\psi_k(\mathbf{r}) = e_k\psi_k(\mathbf{r}),$$

$$U_q(\mathbf{r}) = U_q^{(\mathrm{c})}(\mathbf{r}) + \delta_{q,1}U_C(\mathbf{r}) + \boxed{\mathbf{U}_q^{(\mathrm{s.o.})}(\mathbf{r})\cdot(-i)(\nabla\times\sigma)}.$$

central term, Coulomb term, spin-orbit term

$$U_{\mathrm{HO}}(\mathbf{r}) = \frac{1}{2}M\omega^2r^2.$$

external field for neutron(-proton) drops

Skyrme Functional

- Spin-orbit term

$$\mathbf{U}_q^{(\mathrm{s.o.})}(\mathbf{r}) = \frac{1}{2}\left[W_0 \nabla \rho + W_0' \nabla \rho_q\right] + \left[\alpha \mathbf{J}_q + \beta \mathbf{J}_{1-q}\right],$$

F. Stancu, D. M. Brink, and H. Flocard, Phys. Lett. B 68, 108 (1977)

where

D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972)

$$\rho_q(\vec{\mathbf{r}}) = \sum_{i,\sigma} |\phi_i(\vec{\mathbf{r}}, \sigma, q)|^2,$$

$$\vec{\mathbf{J}}_q(\vec{\mathbf{r}}) = (-i) \sum_{i,\sigma,\sigma'} \phi_i^*(\vec{\mathbf{r}}, \sigma, q)[\vec{\nabla}\phi_i(\vec{\mathbf{r}}, \sigma', q) \times \langle\sigma|\vec{\sigma}|\sigma'\rangle].$$

$\mathbf{J}(\mathbf{r})$ -> 0 for spin-saturated system (j> and j< both occupied),

largest for spin-unsaturated system (j> occupied and j< empty).

Numerical Settings

Fitting protocol is based on the successful SAMi functional

X. Roca-Maza, G. Colò, and H. Sagawa, Phys. Rev. C **86**, 031306 (2012)

Set of data and pseudodata:

- Binding energies and charge radii of ^{40}Ca, ^{48}Ca, ^{90}Zr, ^{132}Sn, and ^{208}Pb.
- Spin-orbit splittings of ^{40}Ca (π1d), ^{90}Zr (π1g), ^{208}Pb (π2f)
- Relative change of spin-orbit splittings from neutron-proton drops ^{40}20 (Z = 20, N = 20) to ^{48}20 (Z = 20, N = 28) calculated by RBHF theory using Bonn A interaction.
- Total energy of neutron drops with neutron number N = 8, 20, 40, 50 calculated by RBHF theory

  S. Shen, *et al.*, *PLB* **778**, 344 (2018)
  S. Shen, *et al.*, *PRC* **97**, 054312 (2018)
- We also keep the empirical hierarchy of the spin G_0 and spin-isospin G_0' Landau-Migdal parameters: $G_0' > G_0 > 0$.

New functional is named as SAMi-T

S. Shen, G. Colò, and X. Roca-Maza, Phys. Rev. C **99**, 034322 (2019)

Ground-State Properties – Experimental Data

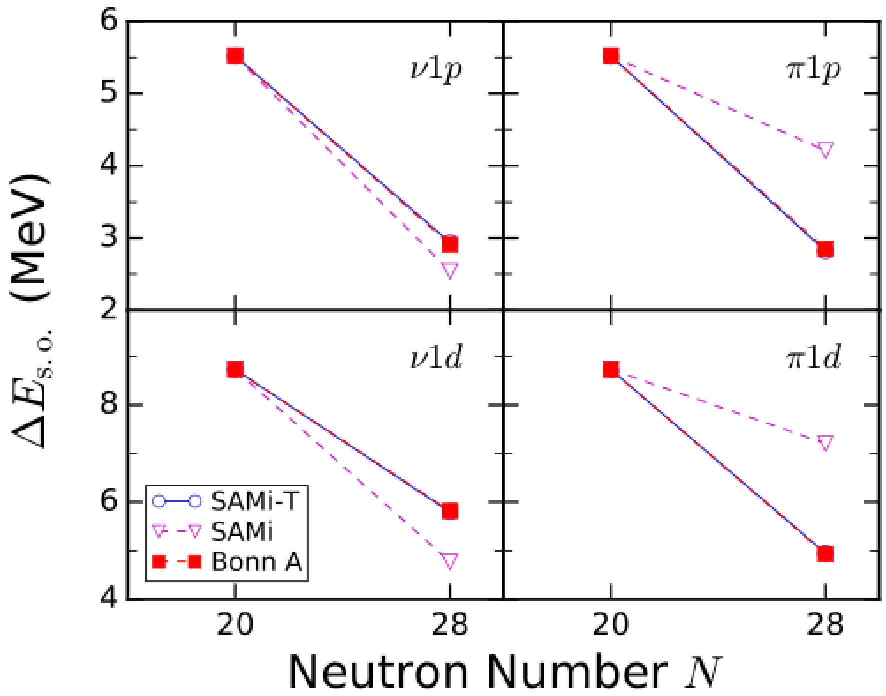
- Binding energy, charge radius, and proton spin-orbit splitting ΔE s.o. (level) of several doubly magic spherical nuclei calculated by using SAMi-T

El.	A	B (MeV)	B^{expt} (MeV)	r_c (fm)	r_c^{expt} (fm)
O	16	127.78(33)	127.62	2.774(4)	2.699
Ca	40	343.74(52)	342.05	3.477(3)	3.478
	48	415.32(50)	415.99	3.515(3)	3.477
Ni	56	468.73(1.06)	483.99	3.784(4)	
	68	591.27(56)	590.41	3.901(4)	
Zr	90	783.35(46)	783.89	4.263(3)	4.269
Sn	100	812.91(1.18)	824.79	4.480(5)	
	132	1100.80(54)	1102.85	4.714(4)	4.709
Pb	208	1637.81(67)	1636.43	5.479(5)	5.501

- χ^2 of SAMi-T are 9.7, 20.1, 11.4 for binding, radius, and SO splitting, respectively.
- Those of SAMi are 32.5, 13.4, 19.0.

Ground-State Properties – Pseudodata

- Neutron and proton 1p and 1d spin-orbit splittings of neutron-proton drops calculated by SAMi-T, in comparison with results of SAMi functional and RBHF theory using the Bonn A interaction.



	α	β
SAMi-T	73.0	101.8
SAMi	101.6	31.5

- The relative change of SO splittings in neutron-proton drops by RBHF can be well fitted by SAMi-T.

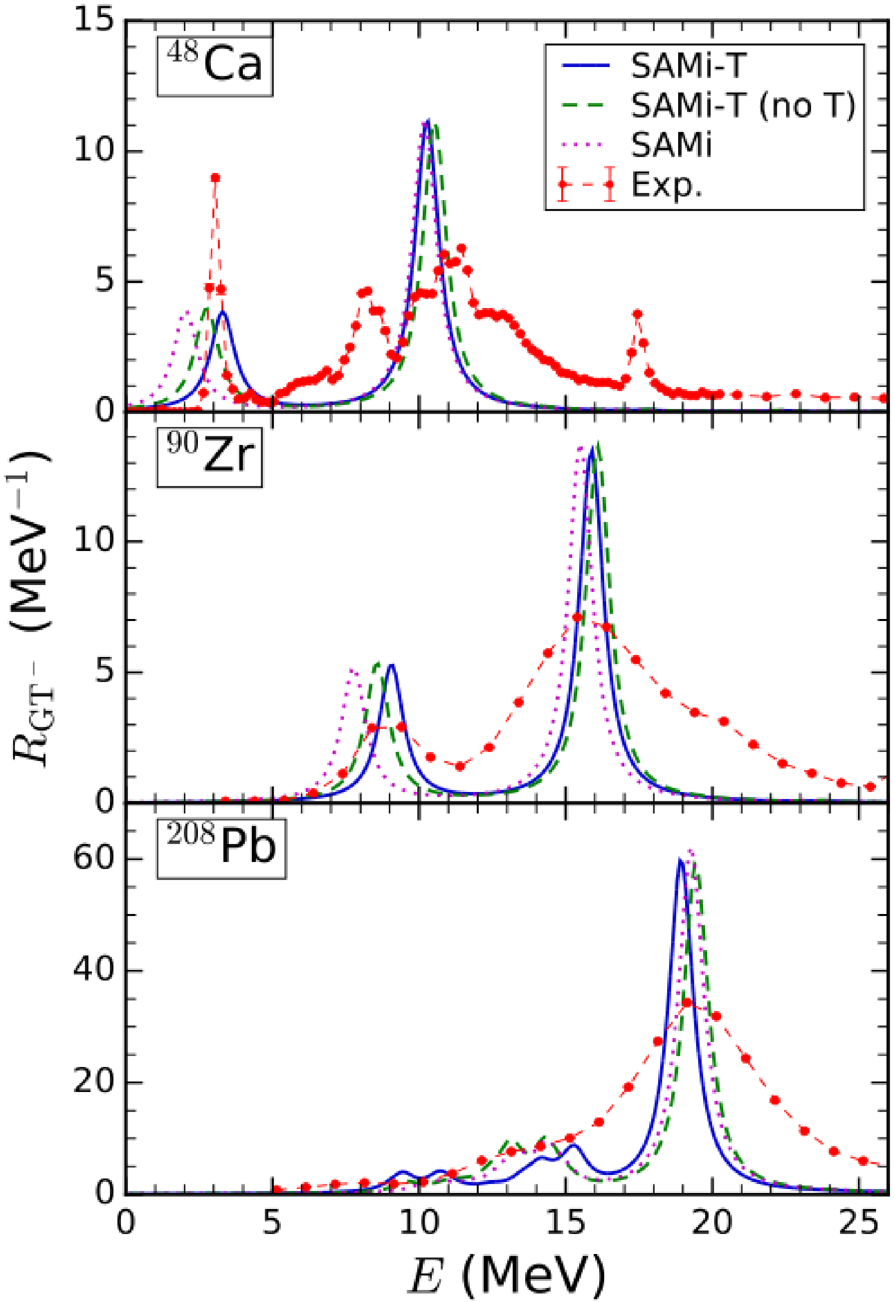
Excited-State Properties – Gamow-Teller

- Gamow-Teller resonance (GTR) strength function for ^{48}Ca, ^{90}Zr, and ^{208}Pb calculated by SAMi-T with and without tensor using self-consistent Hartree-Fock plus Random Phase Approximation.

Exp.

K. Yako, et al., Phys. Rev. Lett. **103**, 012503 (2009)
T. Wakasa, et al., Phys. Rev. C **55**, 2909 (1997)
T. Wakasa, et al., Phys. Rev. C **85**, 064606 (2012)

- Tensor force has little influence.
- SAMi-T gives very good description for the three selected nuclei, both lower and higher peaks.



Excited-State Properties – Spin-Dipole

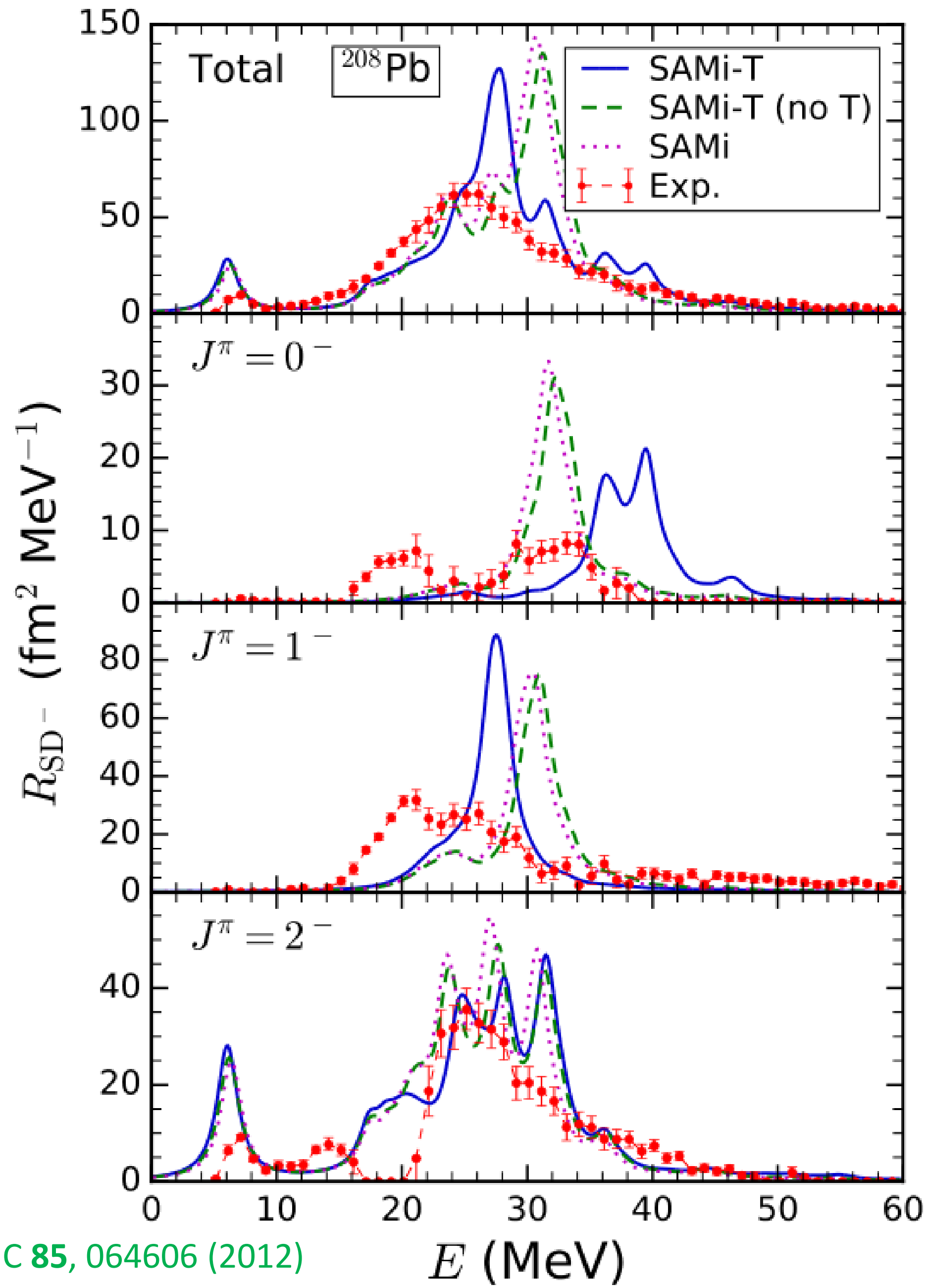
- Spin-dipole resonance (SDR) strength function in the τ− channel for ^{208}Pb.

$$V_{\rm TE}^{(\lambda)} = -\frac{5}{12}T\begin{Bmatrix} 1 \\ -1/6 \\ 1/50 \end{Bmatrix}|\langle p||\hat{O}_{1,\lambda}||h\rangle|^2$$

$$\text{for} \quad \lambda = \begin{Bmatrix} 0^- \\ 1^- \\ 2^- \end{Bmatrix}.$$

C. L. Bai, *et al.*, Phys. Rev. Lett. **105**, 072501 (2010)

- Results of SAMi-T without tensor is similar to those of SAMi.
- Tensor force is important in improving the description of $J^\pi = 1^-$ channel, and improving the total SDR. Consistent with the finding in C. L. Bai, *et al.*, Phys. Rev. Lett. **105**, 072501 (2010)
- Without fitting tensor to SDR, SAMi-T improves the results automatically.



Exp. T. Wakasa, et al., Phys. Rev. C **85**, 064606 (2012)

Summary and Perspectives

Summary

- New Skyrme functional SAMi-T has been developed with tensor force guided by relativistic Brueckner-Hartree-Fock calculations of neutron-proton drops.
- Nuclear ground state properties such as binding energy, radius, and spin-orbit splittings can be well fitted.
- Excited properties like giant monopole, giant dipole, Gamow-Teller, and spin-dipole resonance can be well described by SAMi-T, especially the description for SDR is improved by the tensor force.

Perspectives

- To test the new functional in more studies.
- To study the effect of particle vibration coupling.
- … …

THANK YOU!

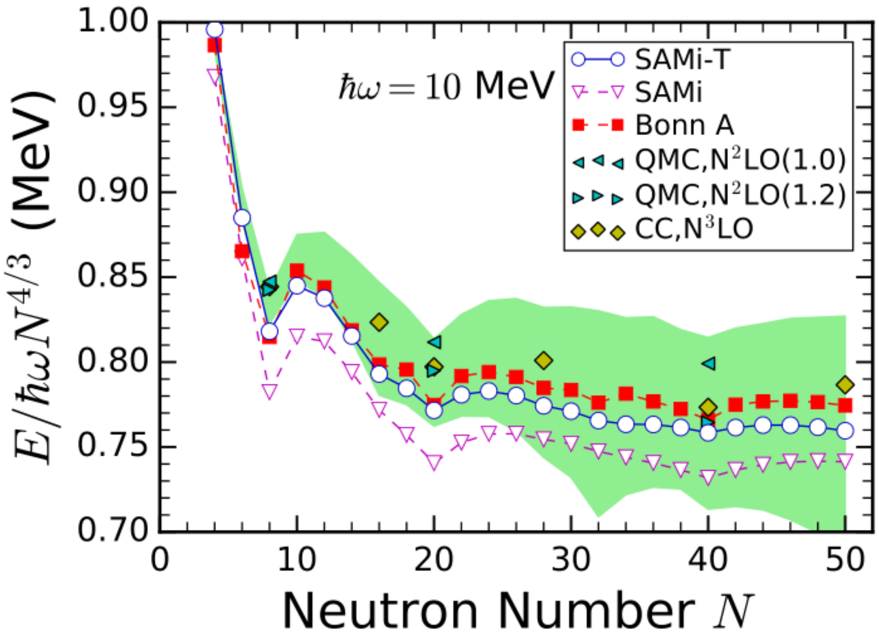
APPENDIX

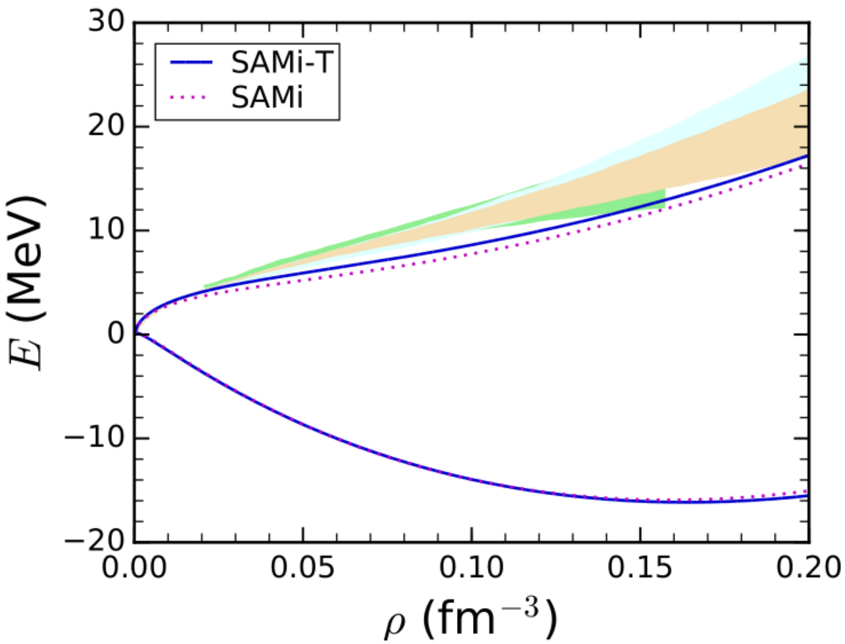
	Value	Error		Value
t_0	-2199.38 MeV fm^3	372.	ρ_0	0.164(1) fm^{-3}
t_1	533.036 MeV fm^5	20.7	e_0	$-16.15(3)$ MeV
t_2	-88.1692 MeV fm^5	12.6	m^*_{IS}/m	0.634(19)
t_3	11293.5 MeV fm$^{3+3\gamma}$	2014.	m^*_{IV}/m	0.625(122)
x_0	0.514710	0.178	J	29.7(6) MeV
x_1	-0.531674	0.593	L	46(12) MeV
x_2	-0.026340	0.117	K_0	244(5) MeV
x_3	0.944603	0.481	G_0	0.08 (fixed)
γ	0.179550	0.047	G_0'	0.29 (fixed)
W_0	130.026 MeV fm^5	8.2		
W_0'	101.893 MeV fm^5	18.6		
α_T	-39.8048 MeV fm^5	39.[illegible]		
β_T	66.6505 MeV fm^5	39.[illegible]		

	Value (σ)		Value (σ)
t_0	$-1877.75(75)$ MeV fm^3	ρ_∞	0.159(1) fm^{-3}
t_1	475.6(1.4) MeV fm^5	e_∞	$-15.93(9)$ MeV
t_2	$-85.2(1.0)$ MeV fm^5	m^*_{IS}	0.6752(3)
t_3	10219.6(7.6) MeV fm$^{3+3\alpha}$	m^*_{IV}	0.664(13)
x_0	0.320(16)	J	28(1) MeV
x_1	$-0.532(70)$	L	44(7) MeV
x_2	$-0.014(15)$	K_∞	245(1) MeV
x_3	0.688(30)	G_0	0.15 (fixed)
W_0	137(11)	G_0'	0.35 (fixed)
W_0'	42(22)		
α	0.25614(37)		

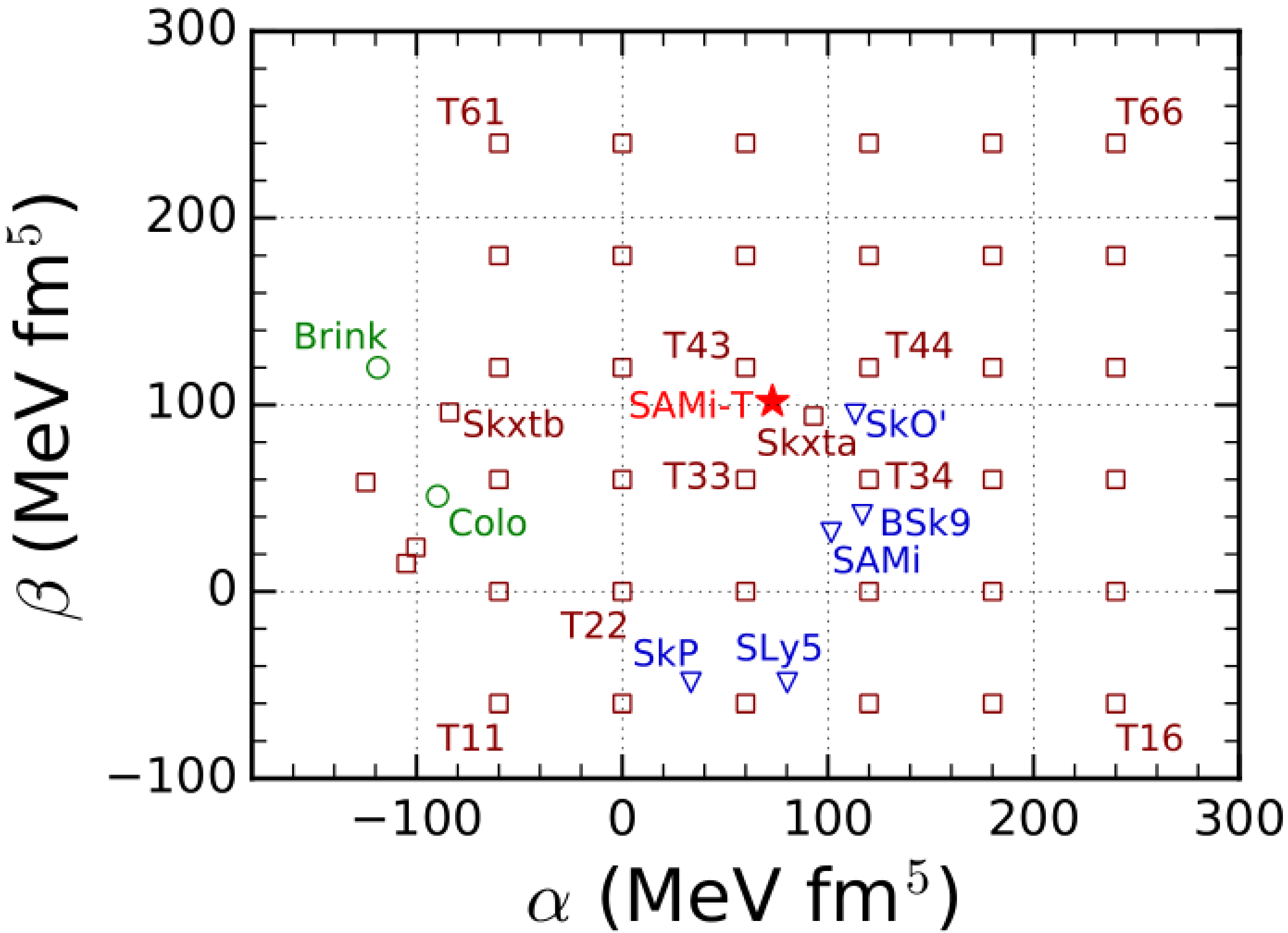
Ground State Properties – Pseudodata (Energy)

- (Left) Energy of neutron drops. (Right) Equation of state of symmetric nuclear matter and pure neutron matter.





- SAMi-T slightly improves the description of pure neutron system than SAMi.



300
200
100
0
−100
−100
0
100
200
300
β (MeV fm^5)
α (MeV fm^5)
T61
T66
Brink
T43
T44
SAMi-T
Skxtb
Skxta
SkO'
T33
T34
Colo
BSk9
SAMi
T22
SkP
SLy5
T11
T16

Skyrme Functional

- Spin-orbit term

$$\mathbf{U}_q^{(\mathrm{s.o.})}(\mathbf{r}) = \frac{1}{2}\left[W_0 \nabla \rho + W_0' \nabla \rho_q\right] + \left[\alpha \mathbf{J}_q + \beta \mathbf{J}_{1-q}\right],$$

F. Stancu, D. M. Brink, and H. Flocard, Phys. Lett. B 68, 108 (1977)

where

$$\rho_q(\vec{r}) = \sum_{i,\sigma} |\phi_i(\vec{r},\sigma,q)|^2,$$

D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972)

$$\vec{J}_q(\vec{r}) = (-i) \sum_{i,\sigma,\sigma'} \phi_i^*(\vec{r},\sigma,q)[\vec{\nabla}\phi_i(\vec{r},\sigma',q) \times \langle\sigma|\vec{\sigma}|\sigma'\rangle].$$

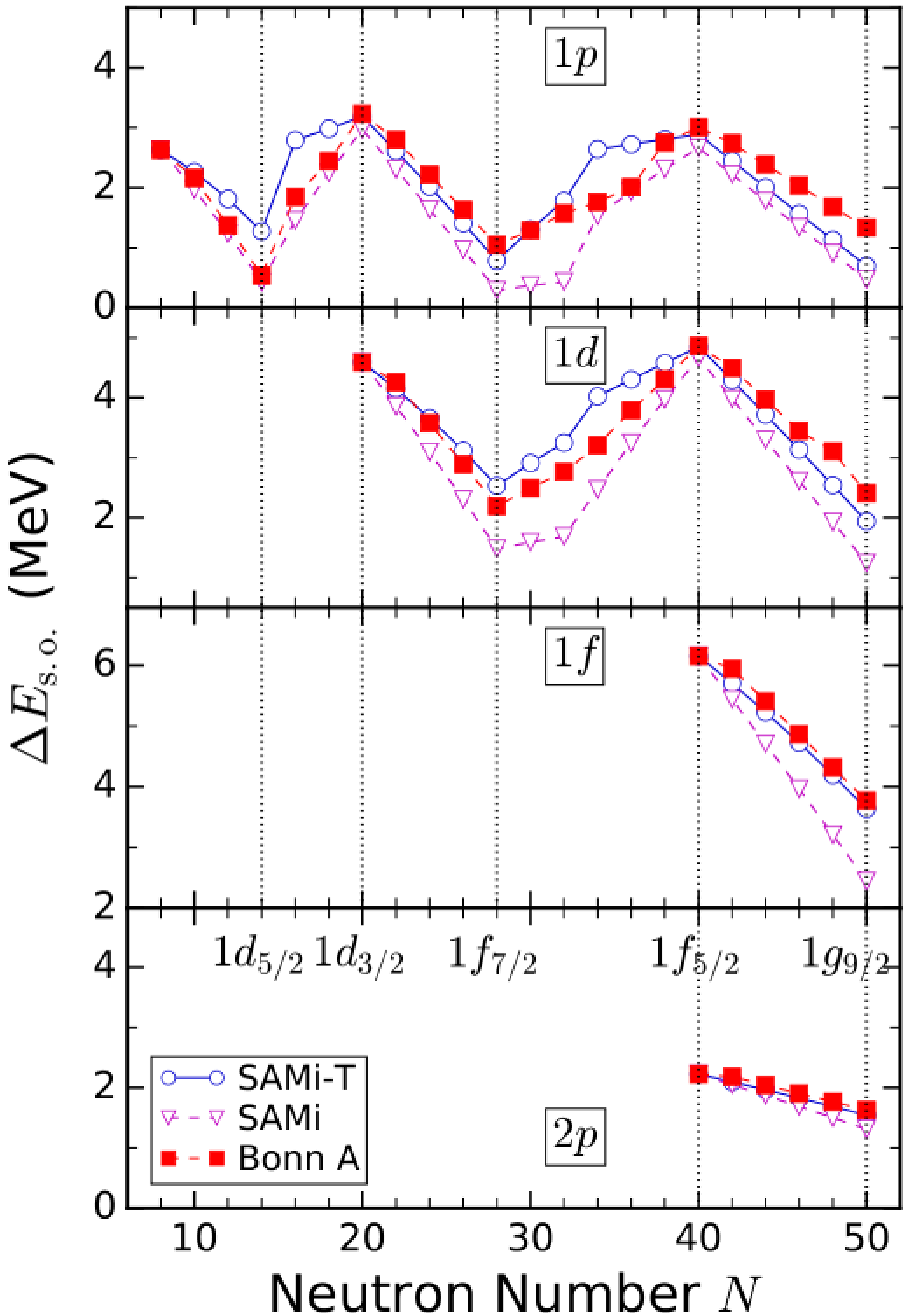
$\mathbf{J}(\mathbf{r})$ -> 0 for spin-saturated system (j> and j< both occupied),
largest for spin-unsaturated system (j> occupied and j< empty).

- Tensor force make contribution through the $\mathbf{J}^2$ term, which is mixed with the contribution from central term

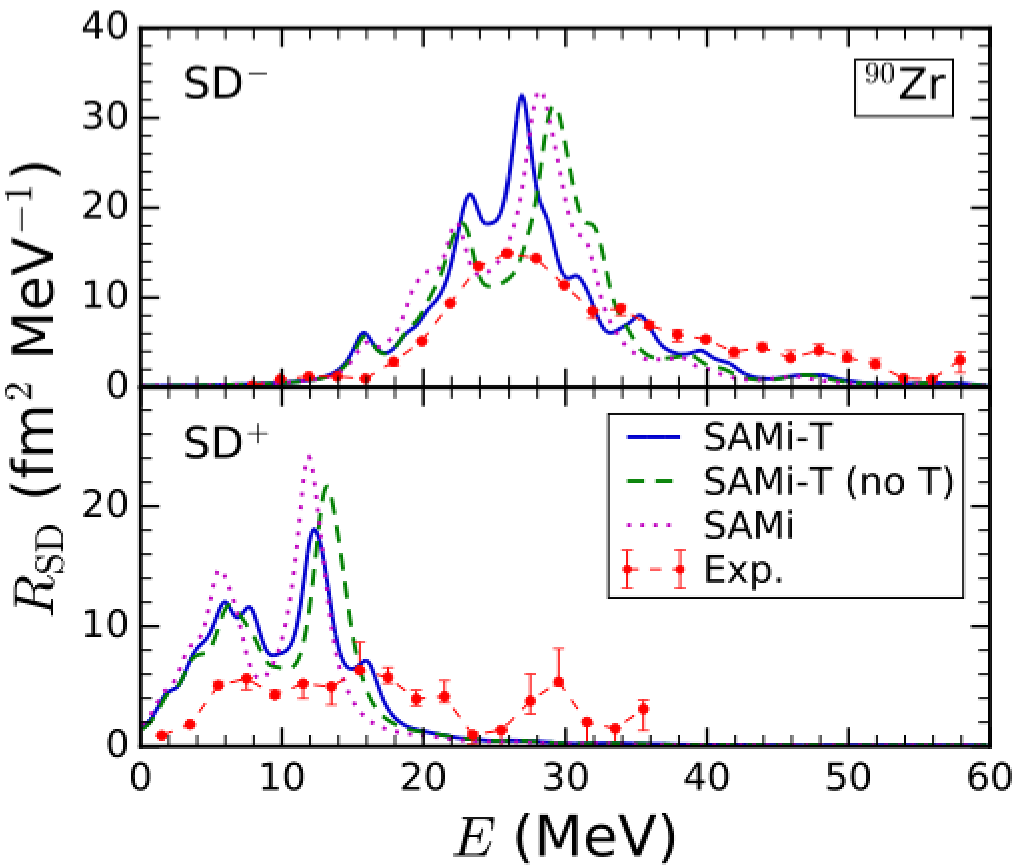
$$\alpha = \alpha_c + \alpha_T, \quad \beta = \beta_c + \beta_T.$$

$$\alpha_c = \frac{1}{8}(t_1 - t_2) - \frac{1}{8}(t_1 x_1 + t_2 x_2), \quad \alpha_T = \frac{5}{12}U,$$

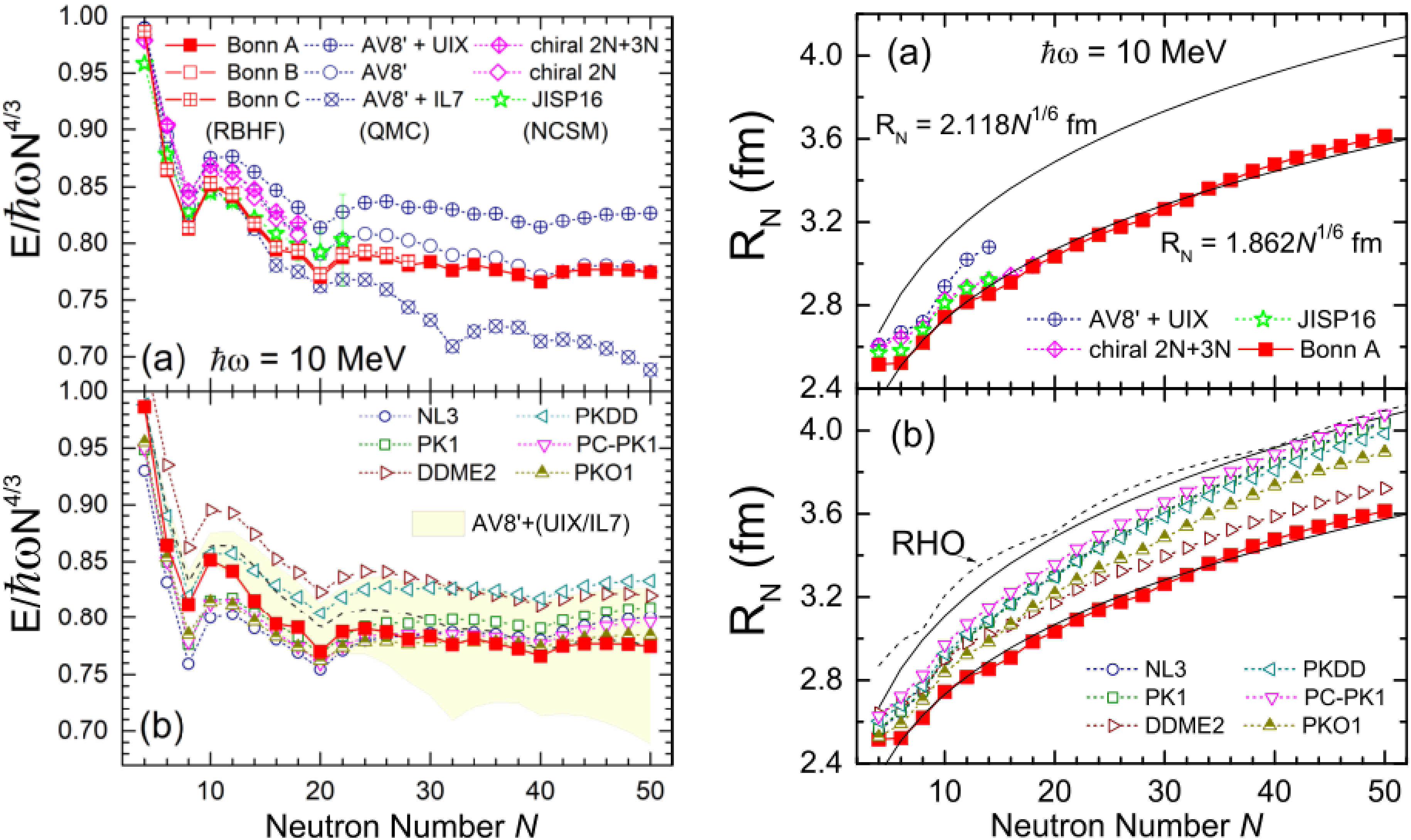
$$\beta_c = -\frac{1}{8}(t_1 x_1 + t_2 x_2), \quad \beta_T = \frac{5}{24}(T + U).$$



1p
1d
1f
2p
$\Delta E_{s.o.}$ (MeV)
$1d_{5/2}$ $1d_{3/2}$ $1f_{7/2}$ $1f_{5/2}$ $1g_{9/2}$
SAMi-T
SAMi
Bonn A
Neutron Number N



SD⁻
⁹⁰Zr
SD⁺
SAMi-T
SAMi-T (no T)
SAMi
Exp.
R_{SD} (fm² MeV⁻¹)
E (MeV)
0
10
20
30
40
50
60



E/ħωN^4/3
Bonn A
Bonn B
Bonn C
AV8' + UIX
AV8'
AV8' + IL7
chiral 2N+3N
chiral 2N
JISP16
(RBHF)
(QMC)
(NCSM)
(a) ħω = 10 MeV
NL3
PK1
DDME2
PKDD
PC-PK1
PKO1
AV8'+(UIX/IL7)
(b)
Neutron Number N
R_N (fm)
(a)
ħω = 10 MeV
R_N = 2.118N^1/6 fm
R_N = 1.862N^1/6 fm
AV8' + UIX
chiral 2N+3N
JISP16
Bonn A
(b)
RHO
NL3
PK1
DDME2
PKDD
PC-PK1
PKO1
Neutron Number N