Magnetic excitations based on relativistic energy-density functional theory

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Kenichi Yoshida (Kyoto Univ.)
Nobuo Hinohara (Tsukuba Univ.)

Outline

- Field = theoretical nuclear physics.
- Framework = relativistic energy-density functional (REDF) theory for multi-nucleon systems.
- Method = REDF-based calculations: self-consistent mean-field; random-phase approximation.
- Target = nuclear magnetic-dipole (M1) excitation & nuclear Cooper pairing/superfluidity (for today's talk).
- Conclusion = M1 data can be good reference to improve the nuclear REDF.

Universal model of nuclei = one dream of nuclear physics

Input = arbitrary set(s) of (Z, N).
Z: proton number
N: neutron number

→ **Universal Theory for Nuclei** →

Output = full information on the (Z, N) nucleus, including e.g.
1. Binding energy,
2. Charge and matter radii,
3. Collective excitation,
4. Radioactivity, etc.

Toward this goal, there are several “architypes” in the nuclear theory.

- ✓ QCD ➔ The most fundamental theory of strong interaction. However, it is non-perturbative to calculate the low-energy nuclear properties. In future, with e.g. lattice or AdS/CFT, maybe done?

Phenomenological approaches:

- ✓ Shell model: *E. Caurier et. al., Review of Modern Physics 77, 427 (2005); L. Coraggio et. al., Progress in Particle and Nuclear Physics 62(1), 135182 (2009).*
- ✓ Ab initio calculation: *S.C. Pieper and R.B. Wiringa, “Quantum Monte Carlo calculations of light nuclei“, Annual Review of Nuclear and Particle Science 51, 5390 (2001); B.R. Barrett, P. Navratil, J.P. Vary, Prog. in Part. and Nucl. Phys. 69, 131181 (2013).*
- ✓ Chiral effective field theory: *R. Machleidt and D.R. Entem, Physics Report 503, 1-75 (2011).*

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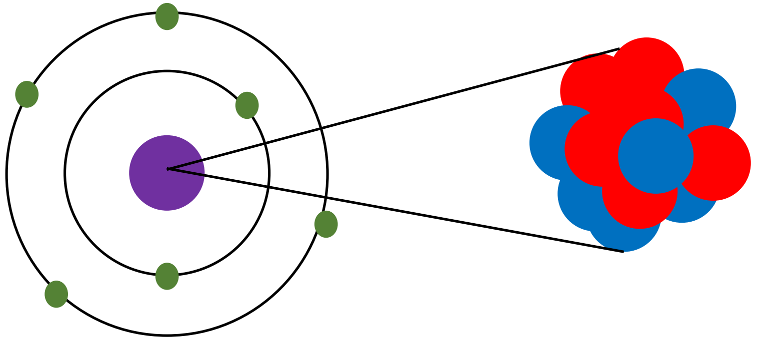
Phenomenological approaches: (continued)

✓ Energy-density functional (EDF) theory for atomic nuclei.
- The practical implementation has been done in the framework of the self-consistent mean-field calculation. The famous example is Hartree-Fock-Bogoliubov (HFB) method.
- Non-relativistic version: Skyrme, Gogny, etc.
- Relativistic version: point-coupling or meson-exchange. ➔ my main interest now.

P.-G. Reinhard, Reports on Progress in Physics 52 (1989) 439.
D. Vretenar, A. V. Afanasjev, G. A. Lalazissis, and P. Ring: Physics Report 409 101 (2005), and references therein.

Atomic nucleus

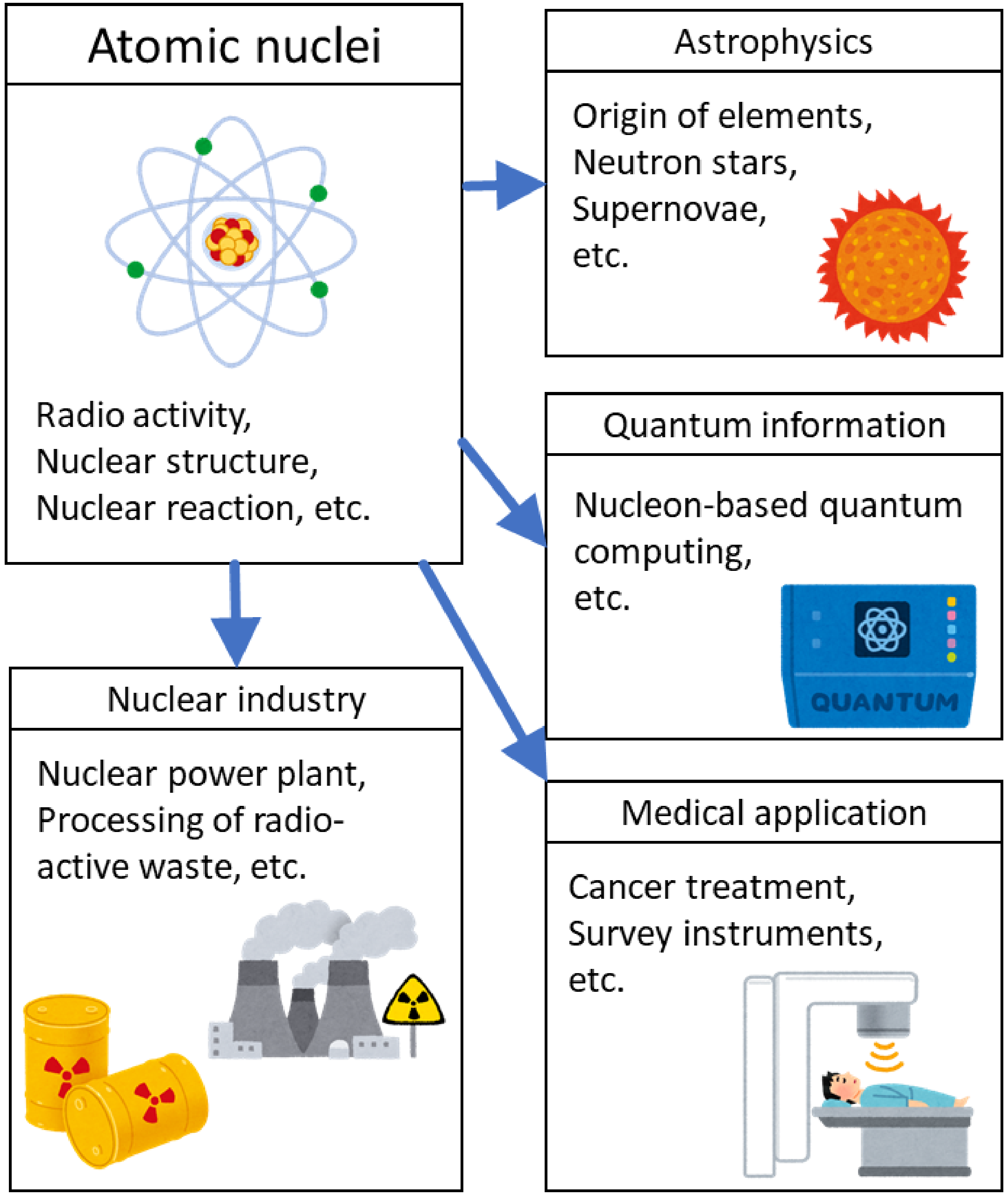
many-body system of protons and neutrons:



The physical properties of atomic nuclei includes,

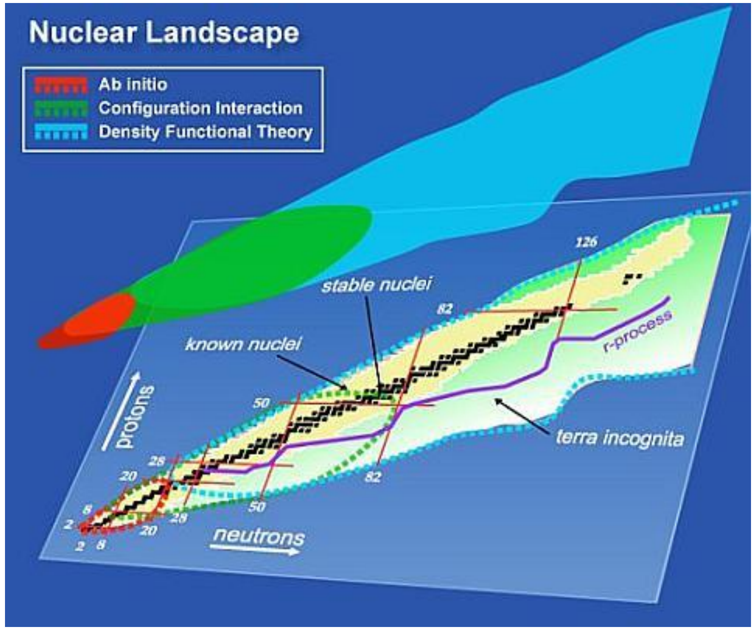
- ✓ Nuclear energy,
- ✓ Nuclear reaction,
- ✓ Radioactivity, etc.

Those properties have been utilized/expected as the basement of various scientific, industrial, and/or technological applications.



EDF-based meanfield calculation

H. Nam et al, J. of Phys. Conf. Series 401, 012033 (2012).



The nuclear EDF theory has been utilized as one tool to calculate the static and dynamical properties widely in the nuclear chart.

- Non-rela' EDF: Skyrme, Gogny, etc.
- Rela' EDF: meson-exchange, point-coupling, etc.

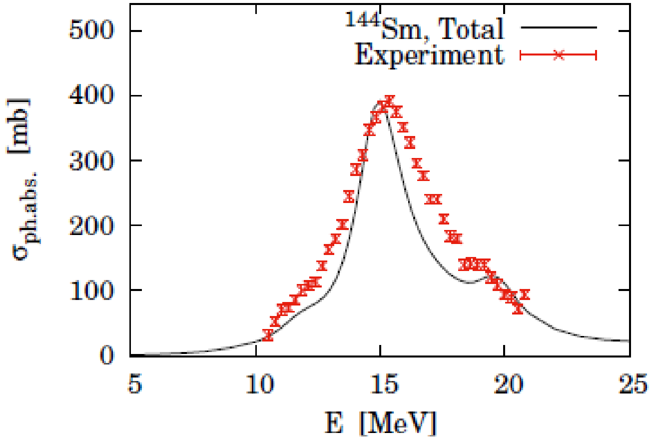
Implementation:

- Static properties (ground state): the self-consistent EDF-meanfield calc.
- Dynamical properties, e.g. collective excitations: the quasi-particle random-phase approximation (QRPA), time-dependent, etc.

QRPA equation (matrix formulation)

$$\hat{\mathcal{H}}\left|\omega\right\rangle = E_\omega \left|\omega\right\rangle, \quad \left|\omega\right\rangle = \hat{\mathcal{Z}}^\dagger(\omega)\left|\Phi\right\rangle \qquad \hat{\mathcal{Z}}^\dagger(\omega) = \frac{1}{2}\sum_{\rho\neq\sigma}\left\{X_{\rho\sigma}(\omega)\hat{\mathcal{O}}^{(J,P)\dagger}_{\sigma\rho} - Y^*_{\rho\sigma}(\omega)\hat{\mathcal{O}}^{(J,P)}_{\sigma\rho}\right\},$$

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix} = \hbar\omega \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix},$$



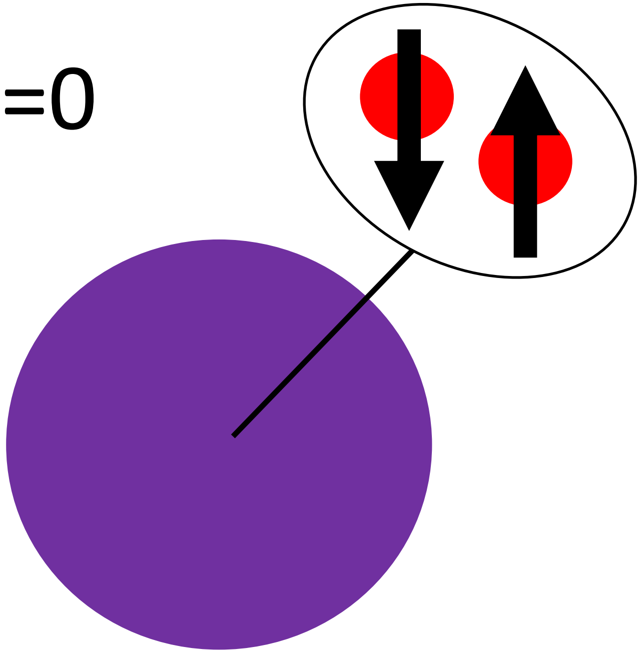
Recent study: Sensitivity of magnetic-dipole (M1) excitation to $S_{12}=0$ and $S_{12}=1$ pairing modes in nuclei

First interest

T.O., G. Kruzic, and N. Paar, Eur. Phys. J. A 57, 1-7 (2021);
T.O., and N. Paar, Phys. Rev. C 100, 024308 (2019).

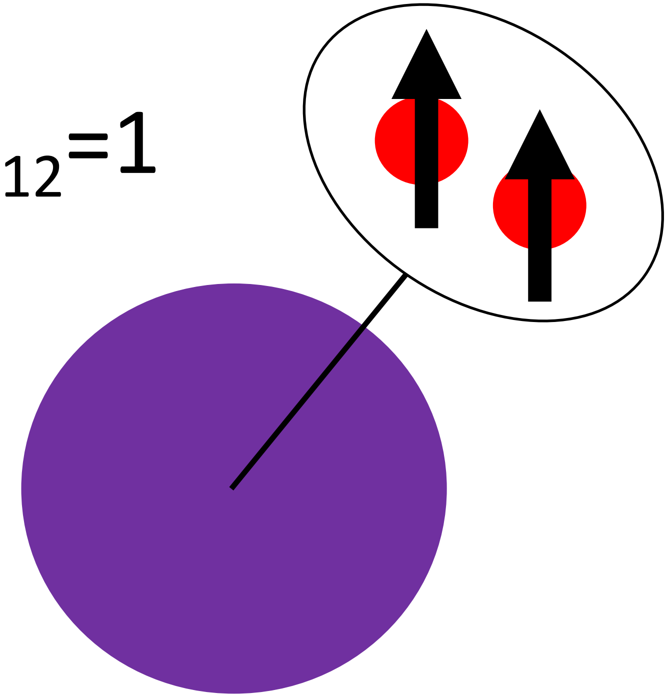
Which mode is dominant? For nuclear super–fluidity?

S_{12}=0



OR/AND

S_{12}=1



Like BCS coupling for electrons

Like Helium-3 superfluidity

➔Usually we assume the S_{12}=0 picture. But is the S_{12}=1 mode unphysical?

Spin-triplet pairing in nuclei

From Hinohara's talk on 2022/Dec/14.

NH, Oishi, Yoshida in preparation

Spin-triplet (S=1) pairing between like-particles (T=1)

two-particle wave function: (space) * (spin) * (isospin)

antisymmetric | symmetric (triplet) | symmetric (triplet)

non-local spin pair density $\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}') = \sum_{ss'} \tilde{\rho}(\boldsymbol{r}st,\boldsymbol{r}'s't)\hat{\boldsymbol{\sigma}}_{s's}$

$\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}') = -\tilde{\boldsymbol{s}}_t(\boldsymbol{r}',\boldsymbol{r})$ antisymmetric in transposition of the coordinates

local (isovector) pair densities generated from non-local spin pair density

tensor pair density $\tilde{\mathsf{J}}_t(\boldsymbol{r}) = \frac{1}{2i}\left[(\boldsymbol{\nabla}-\boldsymbol{\nabla}')\otimes\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}$

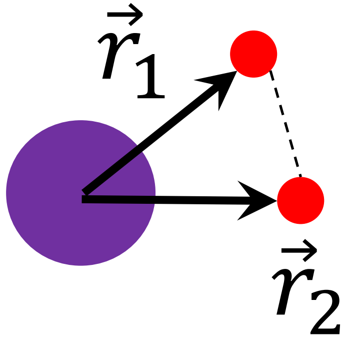
$$
\begin{aligned}
\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}') &= \tilde{\boldsymbol{s}}_t\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\rm rel}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\rm rel}}{2}\right)\\
&= \tilde{\boldsymbol{s}}_t(\boldsymbol{R},\boldsymbol{R}) + \boldsymbol{r}_{\rm rel}\cdot\left[\frac{\partial}{\partial\boldsymbol{r}_{\rm rel}}\otimes\boldsymbol{s}_t\left(\boldsymbol{R}+\frac{\boldsymbol{r}_{\rm rel}}{2},\boldsymbol{R}-\frac{\boldsymbol{r}_{\rm rel}}{2}\right)\Big|_{\boldsymbol{r}_{\rm rel}=0}\right] + \mathcal{O}(|\boldsymbol{r}_{\rm rel}|^2)\\
&= \frac{1}{2}\boldsymbol{r}_{\rm rel}\cdot(\boldsymbol{\nabla}-\boldsymbol{\nabla}')\otimes\tilde{\boldsymbol{s}}_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'=\boldsymbol{R}} + \mathcal{O}(|\boldsymbol{r}_{\rm rel}|^2)\\
&= i\boldsymbol{r}_{\rm rel}\cdot\tilde{\mathsf{J}}_t(\boldsymbol{R}) + \mathcal{O}(|\boldsymbol{r}_{\rm rel}|^2)
\end{aligned}
$$

Spin-triplet pairing in nuclei

T.O. and Nils Paar, PRC 100, 024308 (2019).

Three-body model for ^{42}Ca=^{40}Ca+n+n:

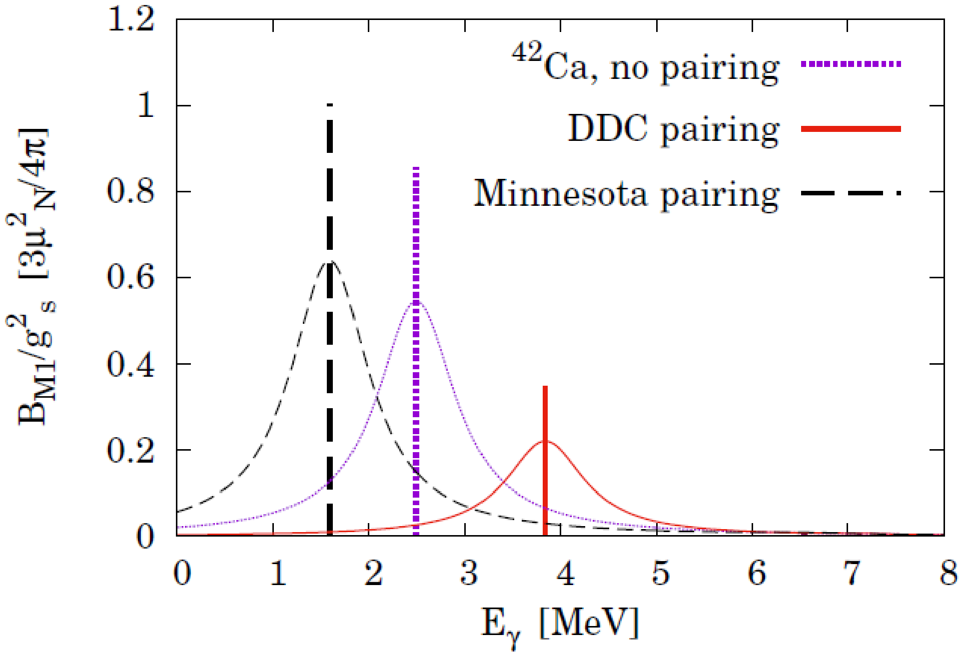
$$H = h_C(1) + h_C(2) + v_{NN}(\boldsymbol{r}_1, \boldsymbol{r}_2) + x_{\rm rec},$$
$$h_C(i) = \frac{p_i^2}{2\mu_i} + V_C(\boldsymbol{r}_i),$$
$$x_{\rm rec} = \frac{\boldsymbol{p}_1 \cdot \boldsymbol{p}_2}{m_C} \quad \text{(recoil term)},$$



	DDC	Minnesota	No pair.
$E_{\rm GS}$	−19.232 MeV	−19.843 MeV	−16.795 MeV
$\langle v_{NN} \rangle$	−2.999 MeV	−3.221 MeV	0 MeV
$\langle x_{\rm rec} \rangle$	−0.005 MeV	−0.012 MeV	0 MeV
$N_{S_{12}=1}$	17.6%	50.6%	42.9%
	(numerical)	(numerical)	(analytic)
SRV	$0.352 g_s^2$	$1.012 g_s^2$	$0.858 g_s^2$
$E_f^{(1)}$	−15.389 MeV	−18.253 MeV	−14.299 MeV
$S_{\rm M1,cal.}$	$0.352 g_s^2$	$1.011 g_s^2$	$0.857 g_s^2$

Note: E_{GS}= $-S_{2n}$= -19.843 MeV in experimental data.

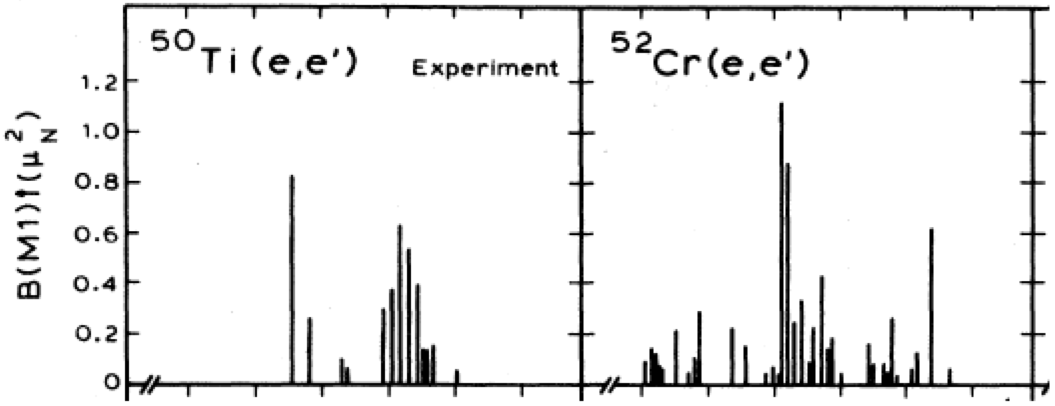
$B_{M1}(E_\gamma;\ 0+ \to 1+)$, $E_\gamma = E_f - E_{GS}$



- ✓ There can be finite ratio of S_{12}=1 pairing.
- ✓ M1 is sensitive to this ratio.

M1 excitation

Magnetic-dipole (M1) mode is one of the excitation modes by the electro-magnetic Interaction, e.g. electron scattering, proton scattering, etc.

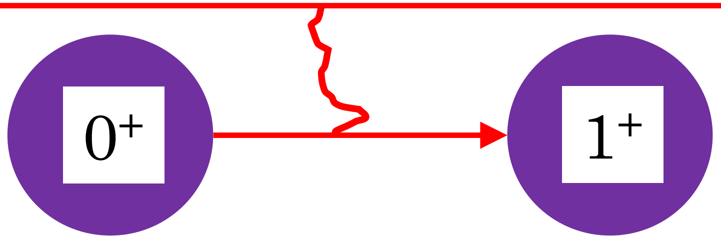


D. I. Sober et al, Phys. Rev. C 31, 2054 (1985).

Selection rule: ΔJ=1, Δπ=0, e.g. 0+(GS) → 1+.

$$\hat{Q}(M1,0) = \mu_{\rm N}\sqrt{\frac{3}{4\pi}}(g_l\hat{l}_0 + g_s\hat{s}_0),$$

$$\hat{Q}(M1,\pm) = (\mp)\mu_{\rm N}\sqrt{\frac{3}{4\pi}}(g_l\hat{l}_\pm + g_s\hat{s}_\pm),$$



For the REDF-residual interactions, which cannot contribute in the even-even ground-state energies, there still remain large ambiguities. For the adjustment of the residual interactions, we need to refer to the measurable process other than the GS.

➔ The M1 response cab be a good reference.

M1 excitation

Matrix elements of M1 up to the 1-body-operator level:

$$\hat{Q}(M1,0) = \mu_{\rm N}\sqrt{\frac{3}{4\pi}}(g_l \hat{l}_0 + g_s \hat{s}_0),$$

$$\hat{Q}(M1,\pm) = (\mp)\mu_{\rm N}\sqrt{\frac{3}{4\pi}}(g_l \hat{l}_\pm + g_s \hat{s}_\pm),$$

M1 operator does not have f(r), and thus, it is expected as sensitive to spin properties.

$$\langle \mathcal{Y}_{l'j'} \| \hat{s} \| \mathcal{Y}_{lj} \rangle = \delta_{l'l}(-)^{l+j'+3/2}\sqrt{(2j'+1)(2j+1)} \begin{Bmatrix} 1/2 & j' & l \\ j & 1/2 & J=1 \end{Bmatrix} \cdot \sqrt{\frac{3}{2}}.$$

$$\left\langle \mathcal{Y}_{l'j'} \| \hat{l} \| \mathcal{Y}_{lj} \right\rangle = (-)^{l'+j+3/2}\sqrt{(2j'+1)(2j+1)} \begin{Bmatrix} l' & j' & 1/2 \\ j & l & J=1 \end{Bmatrix} \cdot \left\langle Y_{l'} \| \hat{l} \| Y_l \right\rangle,$$

$$\text{where } \left\langle Y_{l'} \| \hat{l} \| Y_l \right\rangle = \delta_{l'l}\sqrt{(2l+1)(l+1)l}.$$

→ M1 transition can happen between LS partners, e.g. $f_{7/2}$ → $f_{5/2}$.
Since the nuclear LS splitting is finite, M1 is measurable.

Proton inelastic scattering to probe M1

P. von Neumann-Cosel and A. Tamii, Eur. Phys. J. A 55, 110 (2019):

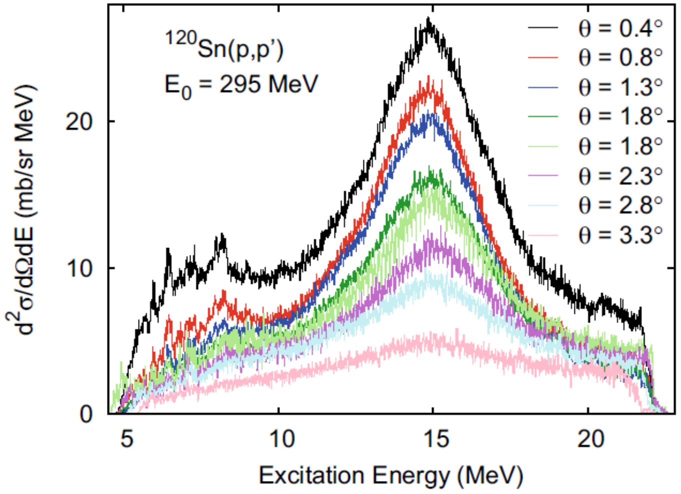


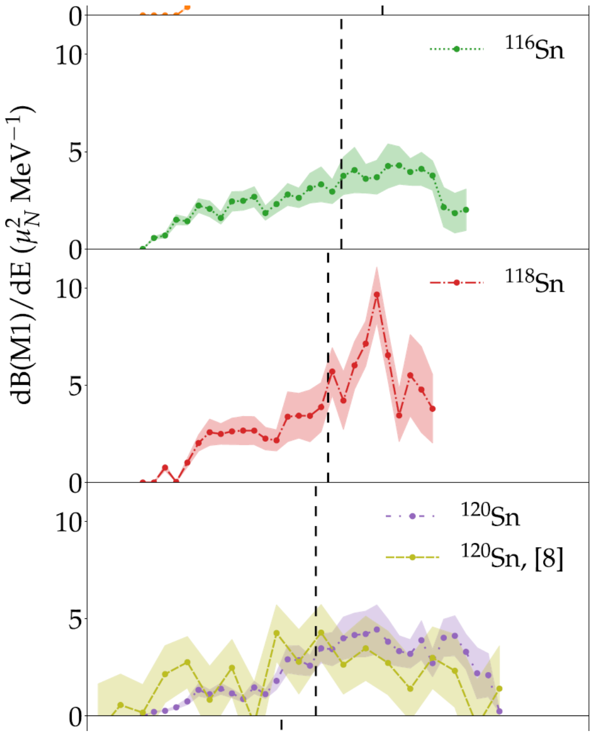
Fig. 11. Experimental cross sections of the ^{120}Sn(p, p′) reaction at E_0 = 295 MeV for different angle cuts. The top four spectra originate from a measurement with the central Grand Raiden spectrometer angle set to 0°, whereas the lower four were taken at 2.5°. Figure taken from ref. [147].

S. Bassauer et. al., Phys. Rev. C 102, 034327 (2020):

M1 data for Sn isotopes are obtained.

TABLE V. Neutron threshold energies S_n, $B(M1)$ strengths up to S_n, and total $B(M1)$ strengths up to energy $E_{\max}$ in ^{112,114,116,118,120,124}Sn deduced from the present data as described in the text.

	S_n (MeV)	$\sum_6^{S_n} B(M1)$ (μ_N^2)	$E_{\max}$ (MeV)	$\sum_6^{E_{\max}} B(M1)$ (μ_N^2)
^{112}Sn	10.79	13.1(1.2)	11.2	14.7(1.4)
^{114}Sn	10.30	9.2(1.0)	12.8	19.6(1.9)
^{116}Sn	9.56	8.1(0.7)	11.8	15.6(1.3)
^{118}Sn	9.32	8.2(1.1)	11.2	18.4(2.4)
^{120}Sn	9.10	4.8(0.5)	12.4	15.4(1.4)
^{124}Sn	8.49	5.6(0.6)	11.4	19.1(1.7)



➔ These new data can be a good reference to examine & improve the REDF framework.

Calculations, results, and discussions

Rela' Hartree-Bogoliubov & QRPA

Point-coupling REDF Lagrangian: $\mathcal{L} = \bar{\psi}(x)[i\gamma_\mu\partial^\mu - M]\psi(x) + \mathcal{L}_{\rm M} + \mathcal{L}_{\rm I}.$

$$\mathcal{L}_I = -\frac{\alpha_{\rm IS-S}(\rho)}{2}[\bar{\psi}\psi][\bar{\psi}\psi] - \frac{\alpha_{\rm IS-V}(\rho)}{2}[\bar{\psi}\gamma_\mu\psi][\bar{\psi}\gamma^\mu\psi] - \frac{\alpha_{\rm IV-V}(\rho)}{2}[\bar{\psi}\gamma_\mu\vec{\tau}\psi][\bar{\psi}\gamma^\mu\vec{\tau}\psi]$$

DD-PC

$$- \frac{\alpha_{\rm IV-PV}(\rho)}{2}[\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi][\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi] - e\bar{\psi}\gamma_\mu A^\mu \left(\frac{1-\hat{\tau}_3}{2}\right)\psi$$

IV-PV for QRPA

- ✓ (i) For the GS of even-even nuclei, the relativistic Hartree-Bogoliubov (RHB) calculation is performed by using the DD-PC setting for Lagrangian [1, 2]. (ii) Two-Gaussian pairing force is employed in the particle-particle channel [3]. (iii) For the M1-excited states, the QRPA is employed [3].

QRPA: $\frac{dB_{\rm M1}}{dE_\gamma} = \sum_i \delta(E_\gamma - \hbar\omega_i) \sum_\nu \left| \left\langle \omega_i \middle| \hat{Q}_\nu({\rm M1}) \middle| \Phi \right\rangle \right|^2$ from $\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix} = \hbar\omega \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix},$

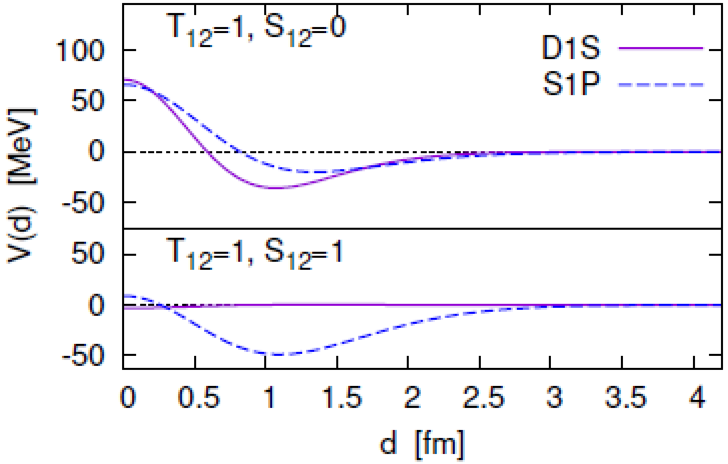
- ✓ (iv) In the QRPA, we additionally consider the IV-PV coupling as the residual interaction [3]. Note that this IV-PV originates in the one-pion exchange. (v) Fock terms (Fiertz transformations) are neglected…

References: *[1] T. Niksic, D. Vretenar, and P. Ring, Progress in Particle and Nuclear Physics 66(3), 519-548 (2011). [2] T. Niksic et. al., Comp. Phys. Com., 107184 (2020). [3] G. Kruzic et. al., PRC 102, 044315 (2020).*

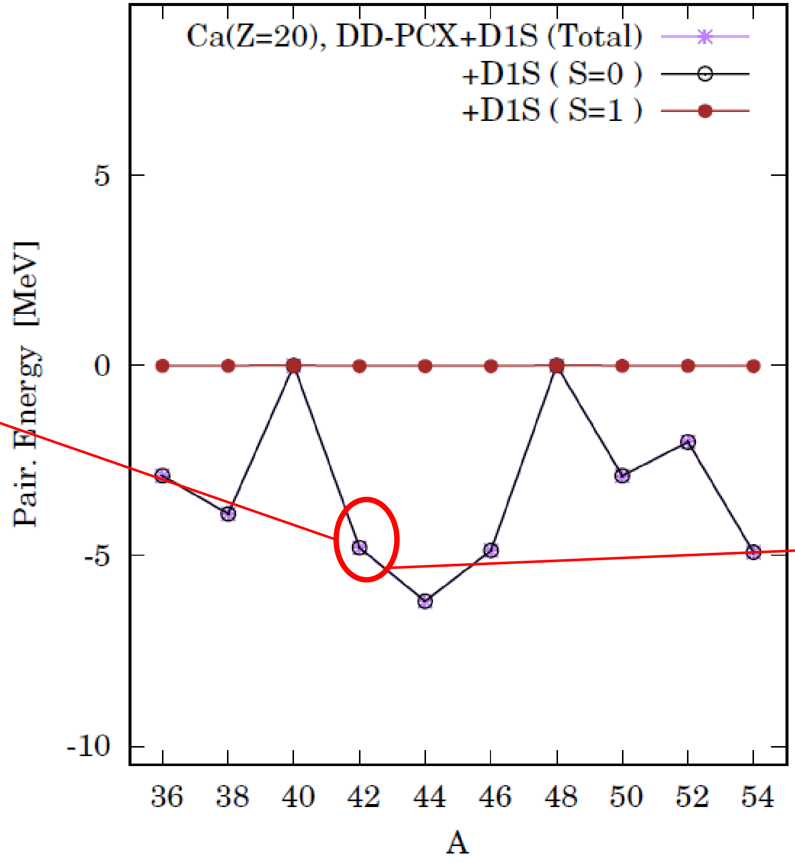
Two pairing models

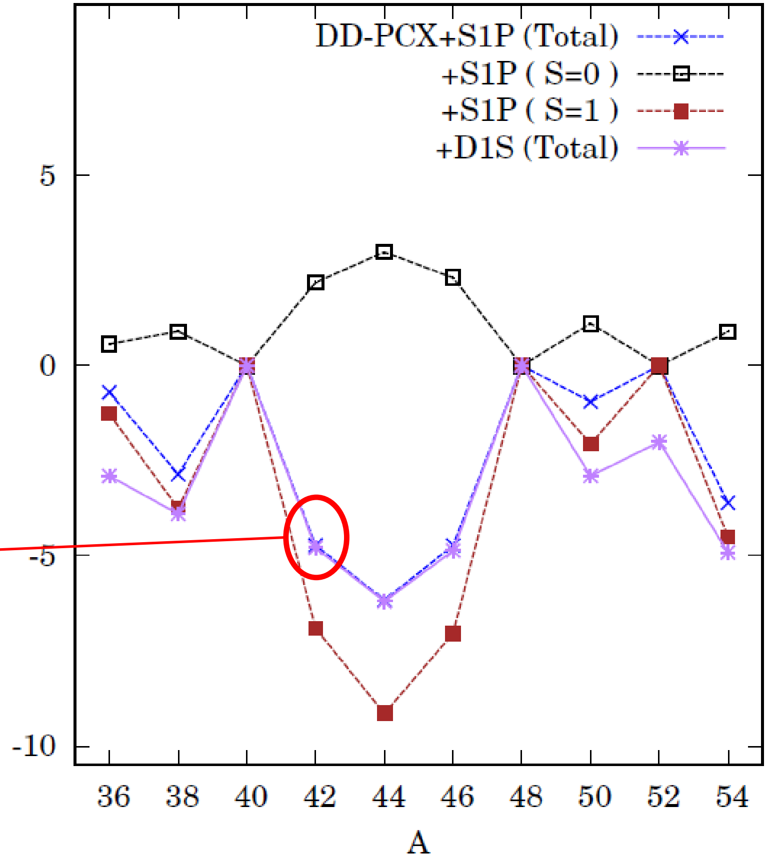
T.O., G. Kruzic, N. Paar, Eur. Phys. J. A 57, 1-7 (2021) +α.

Two pairing models for $S_{12}=0$ and $S_{12}=1$ modes are compared. Those are tuned to equivalently output $\Delta_{pair.}$ = -4.84 MeV for ^{42}Ca.



$$V_{pp} = \sum_{i=a,b} \left\{ (W_i - H_i) + (B_i - M_i)\hat{P}_\sigma \right\} e^{-\frac{d^2}{\mu_i^2}},$$





D1S ➔ $S_{12}=0$ pairing is dominant.
ZM3 ➔ $S_{12}=1$ pairing is dominant (S1P).
For several GS solutions, two models show a different gaps.

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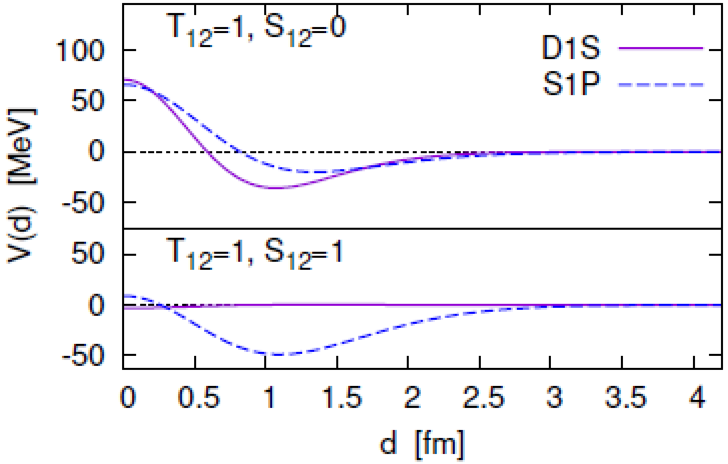

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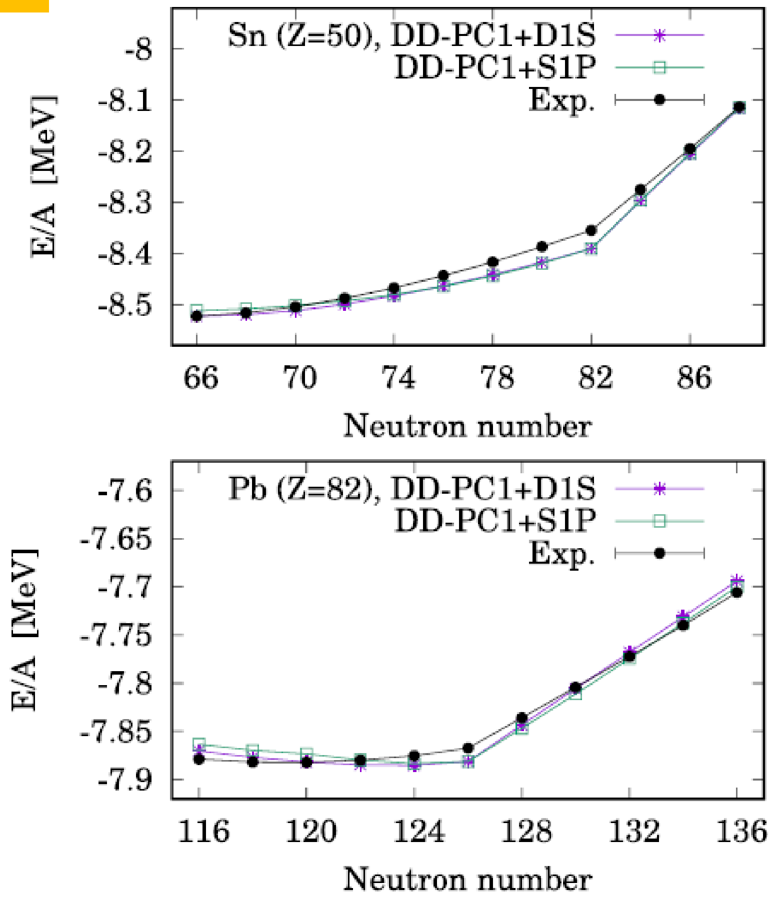

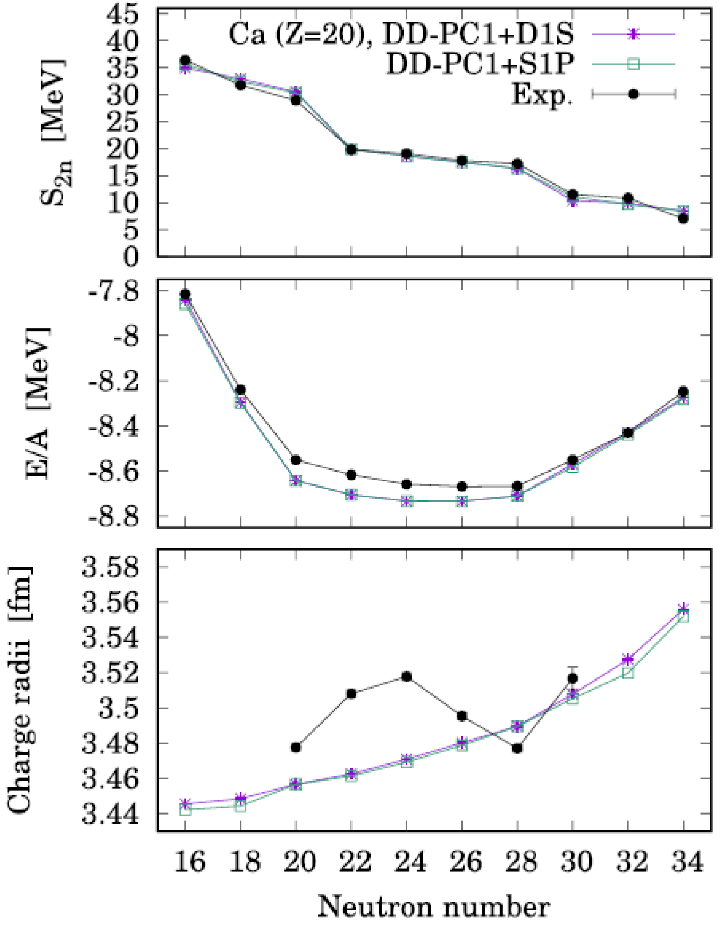

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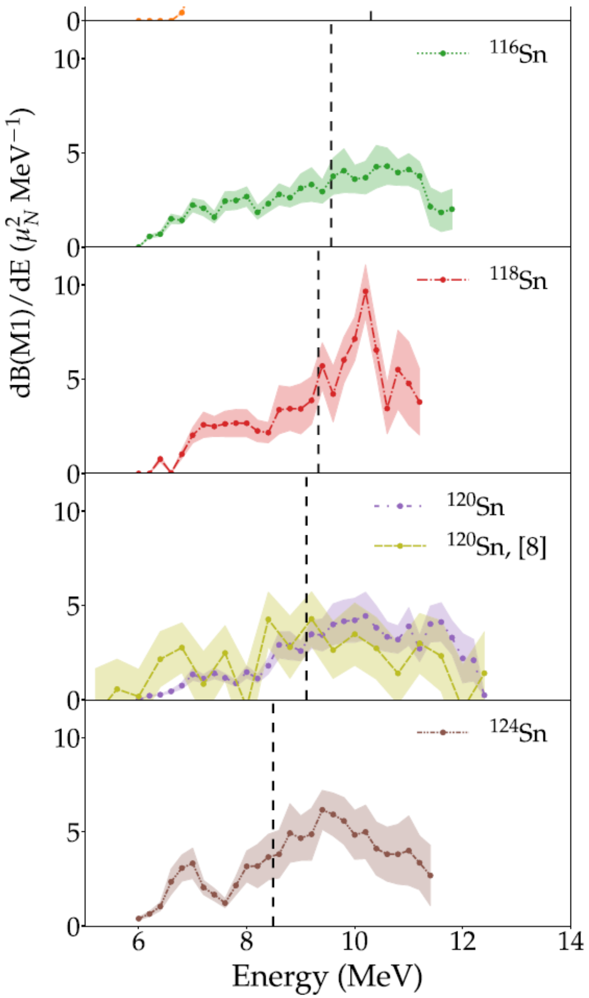
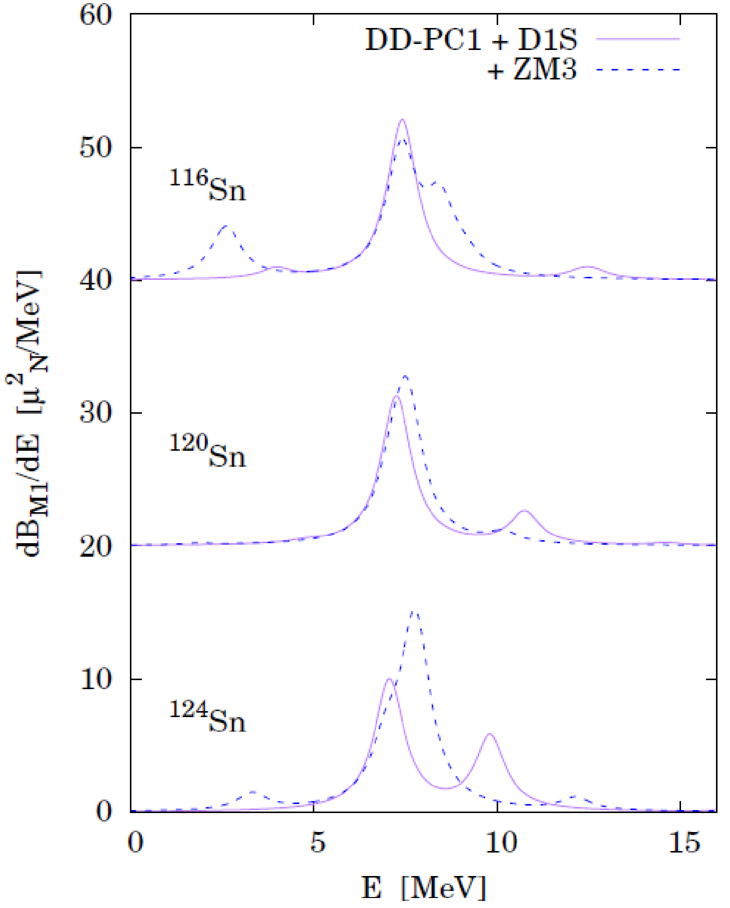
Sensitivity of M1 to pairing models

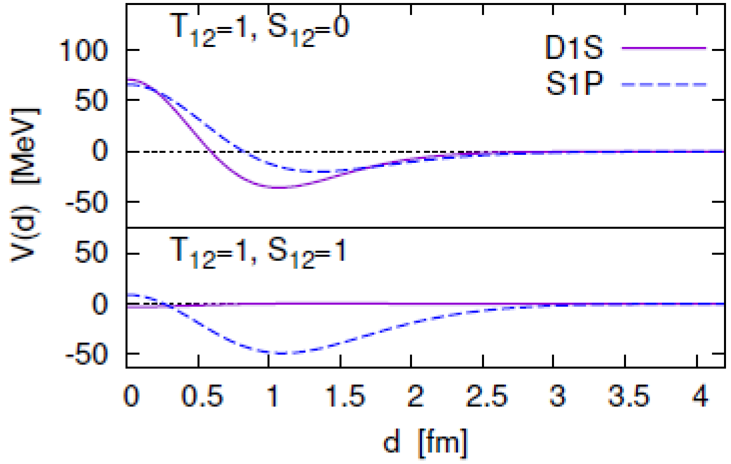
Expt. = S. Bassauer et. al., Phys. Rev. C 102, 034327 (2020):



v.s. our QRPA results:

$$R_{\rm M1}(E) = \sum_{\nu} B_{\rm M1}(\omega_\nu) \frac{1}{\pi} \frac{\Gamma/2}{(E-\hbar\omega_\nu)^2 + (\Gamma/2)^2},$$



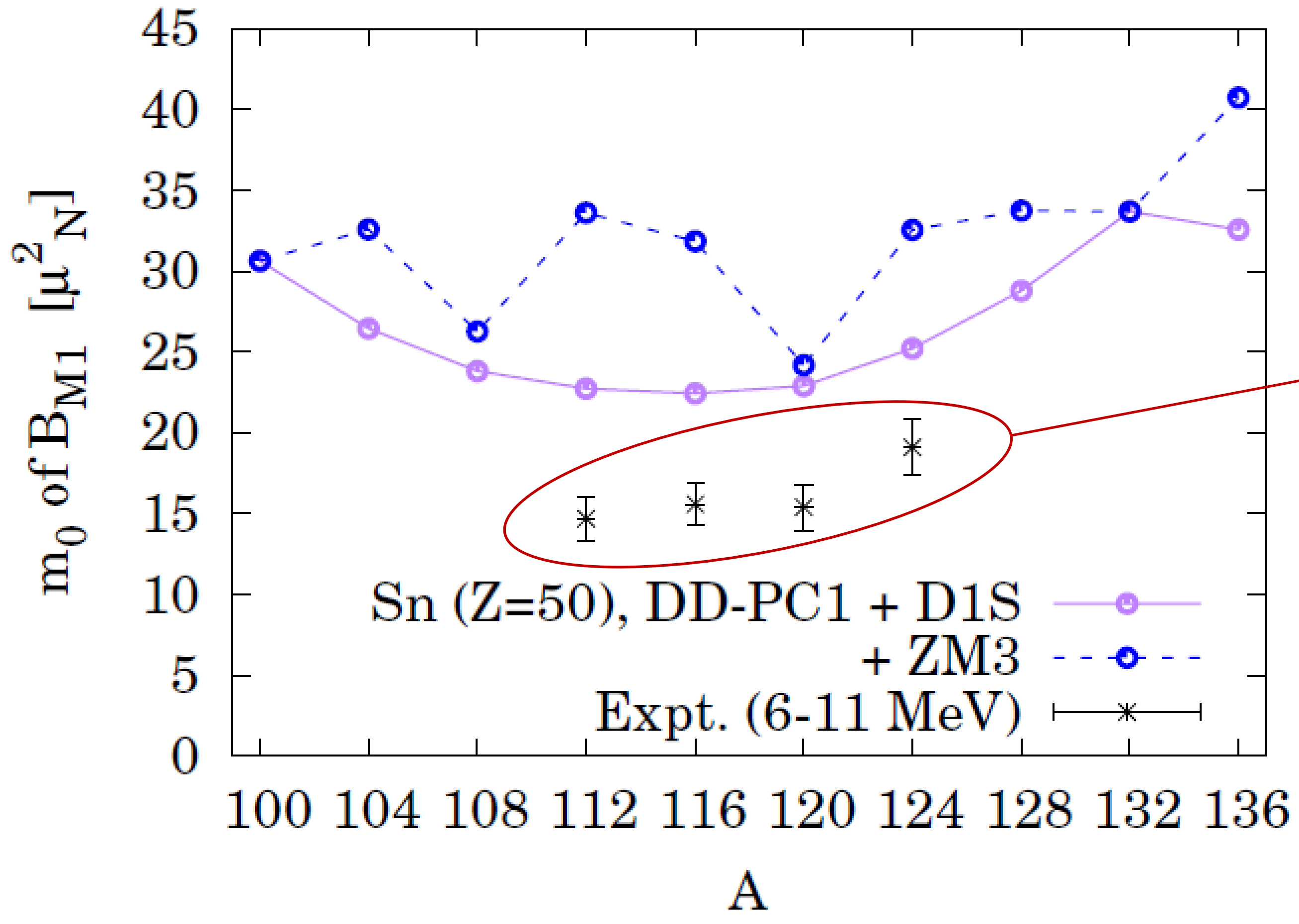


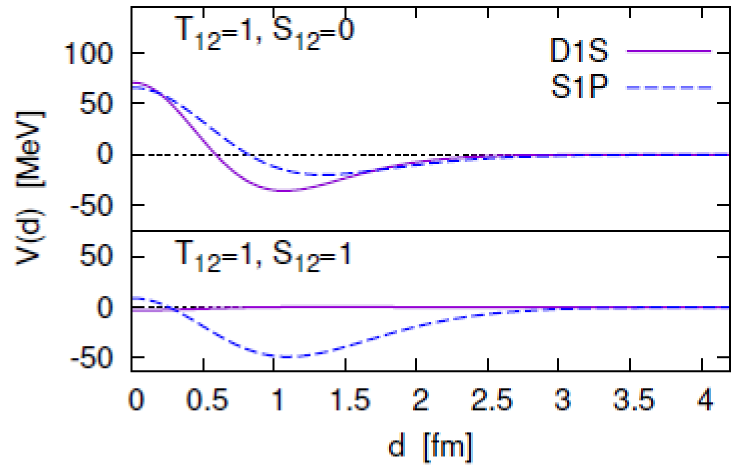
The major M1 energy is reproduced with both models. However, the ZM3(=S1P) predicts the low-lying peak, which is not measured.

➔ D1S looks better.

Sensitivity of M1 to pairing models

m_0 = total summation of $B_{M1}(E)$ for Sn: $m_k(\mathrm{M1}) \equiv \int E_\gamma^k \frac{\mathrm{d}B_{\mathrm{M1}}}{\mathrm{d}E_\gamma}\, \mathrm{d}E_\gamma.$





Experiment = S. Bassauer et. al., Phys. Rev. C 102, 034327 (2020).

Note that the expt. M1 summation is limited without low- and high-energy regions.

S_{12}=0 (D1S) pairing model looks better.
(The S_{12}=0 (ZM3) result looks strange…)

Link of M1 with pairing

T.O., G. Kruzic, N. Paar, J. Phys. G 47, 115106 (2020).

(We only consider the neutron's M1 excitation here.) The 0^{th} summation of M1 is given as

$$m_0 \equiv \sum_{\nu}\sum_{E}\left|\left\langle E\right|\left(g_l\hat{L}_\nu + g_s\hat{S}_\nu\right)\left|i\right\rangle\right|^2$$

$$= \left\langle i\right|\left(g_l\hat{\mathbf{L}} + g_s\hat{\mathbf{S}}\right)^2\left|i\right\rangle. \qquad \hat{L}_\nu = \sum_{k\in N}\hat{l}_\nu^{(k)} \text{ and } \hat{S}_\nu = \sum_{k\in N}\hat{s}_\nu^{(k)}$$

Then, by using the notation J=L+S (total angular momentum),

$$m_0 = g_l(g_l - g_s)\left\langle\hat{\mathbf{L}}^2\right\rangle_{[i]} + g_s(g_s - g_l)\left\langle\hat{\mathbf{S}}^2\right\rangle_{[i]} + g_l g_s\left\langle\hat{\mathbf{J}}^2\right\rangle_{[i]}.$$

For the GS of even-even nuclei with $J_i^P=0^+$, the allowed components are of (L=S), only. Therefore,

$$m_0 = \sum_{(L,S)}\delta_{L,S}\left|C_{(L,S)}\right|^2\left\{g_l(g_l-g_s)\cdot L(L+1) + g_s(g_s-g_l)\cdot S(S+1)\right\}$$

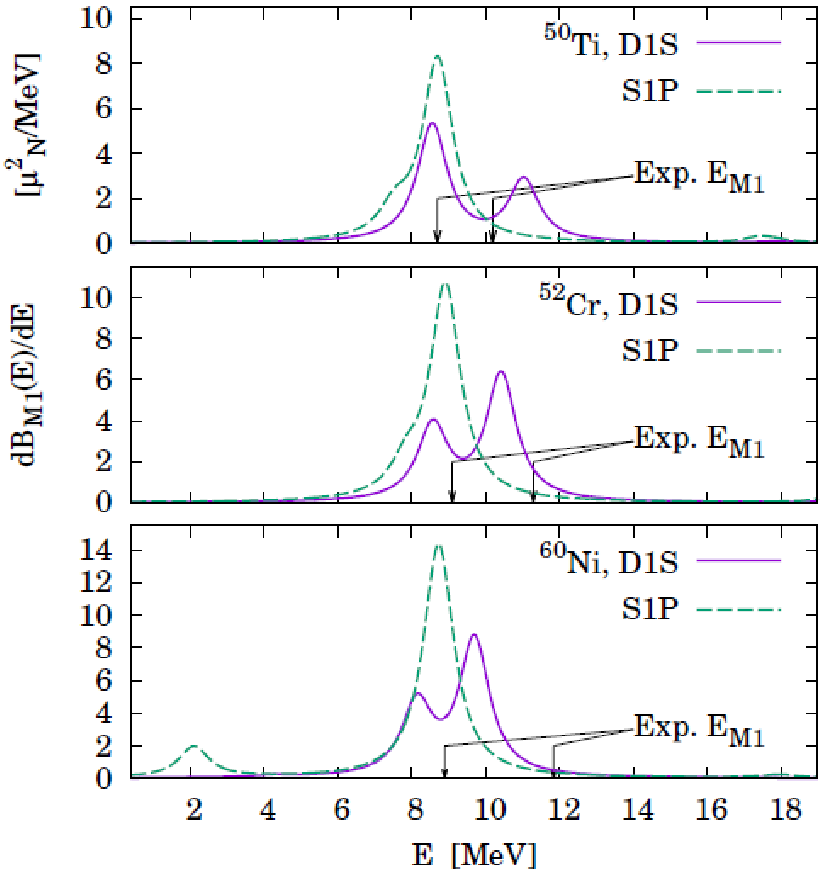
$$= \sum_{S}\left|C_{(L=S,S)}\right|^2(g_l-g_s)^2 S(S+1).$$

If the (s_{12}=0) mode of pairing is dominant, the total spin S is 0, too. ➔ m_0 is small. Otherwise, including the non-zero S components, the m_0 value can be enhanced.

M1 in open-shell nuclei

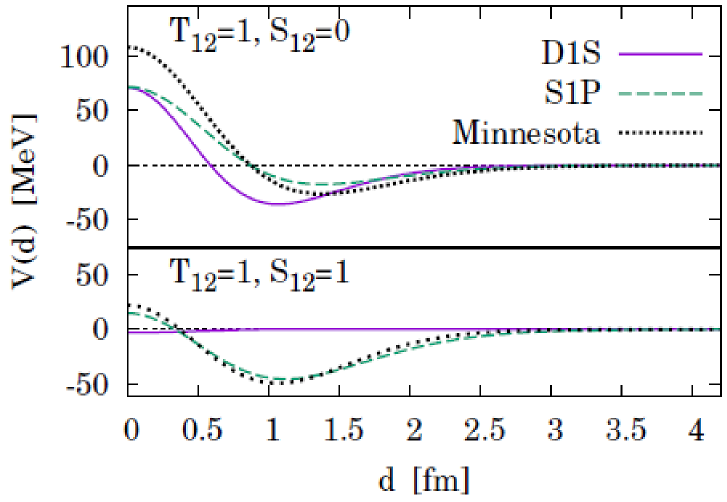
T.O., G. Kruzic, N. Paar, Eur. Phys. J. A 57, 1-7 (2021).

M1 response of open-shell nuclei with DD-PC1 plus IV-PV REDF (Gaussian pair.) for the ph (pp) channel of the relativistic QRPA.



Expt. Data = D. I. Sober, et al, Phys. Rev. C 31, 2054 (1985).

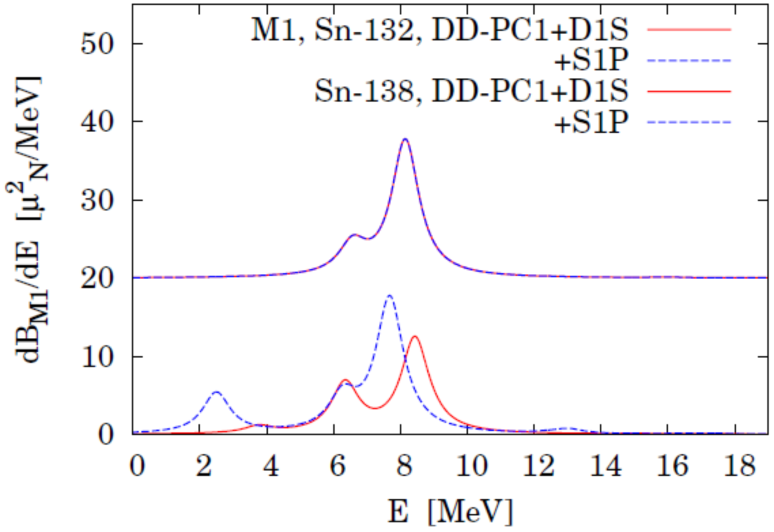
with

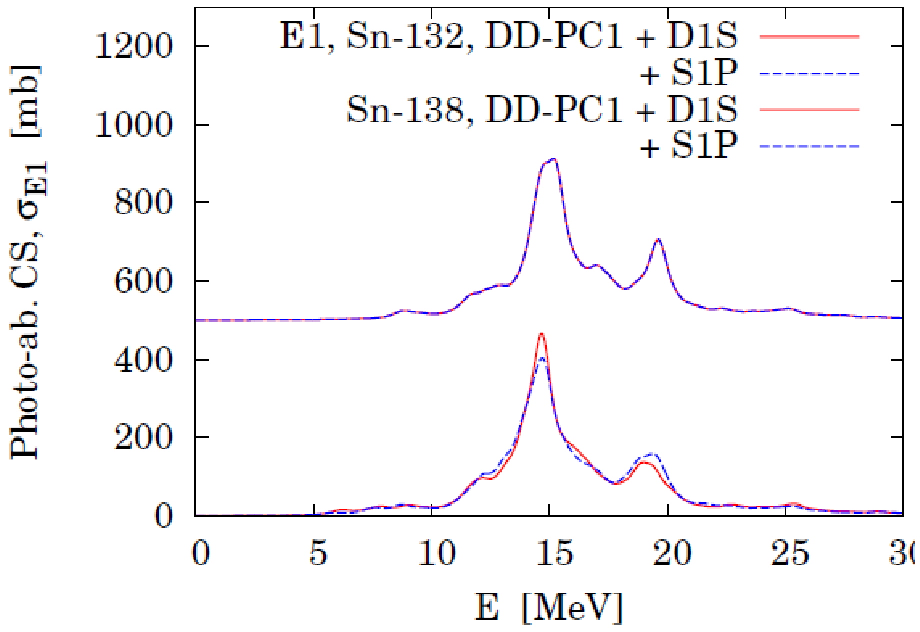


S_{12}=0 looks as the better option to qualitatively reproduce experimental M1 data. S_{12}=1 pairing picture has not been validated in our result.

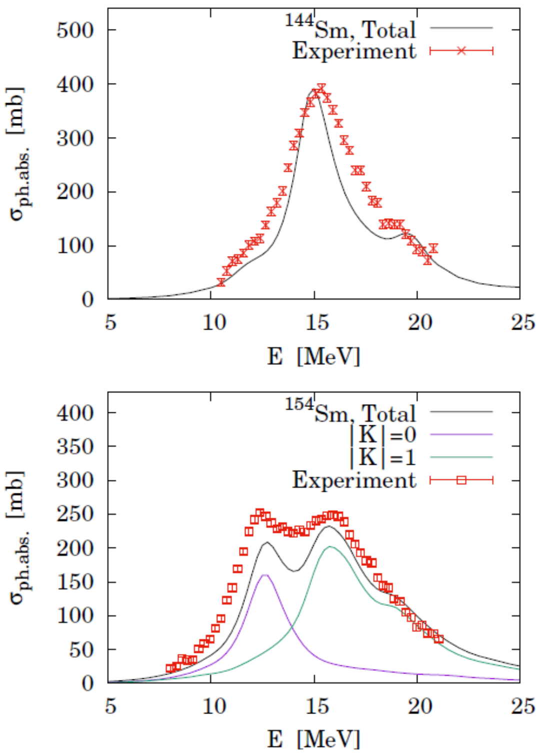
Systematic M1 data can provide an evidence of the Cooper-pairing mode(s) inside nuclei.

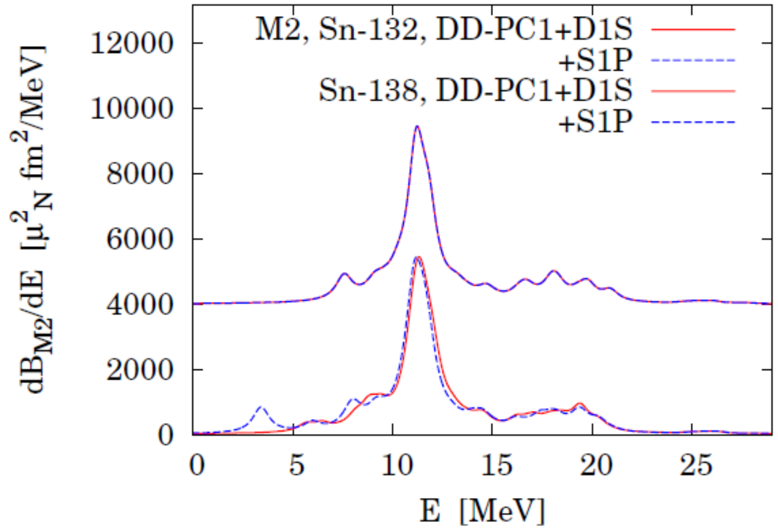
How about it in other E/M modes?





Test of QRPA in E1:





➔ M1 is especially sensitive to pairing modes.

➔ M2 with S1P yields the low-lying resonance.

➔ E1 is not sensitive. This insensitivity is checked also in E2 and E3.

Problem now we face on

T.O., Ante Ravlic, Nils Paar, PRC 105, 064309 (2022).

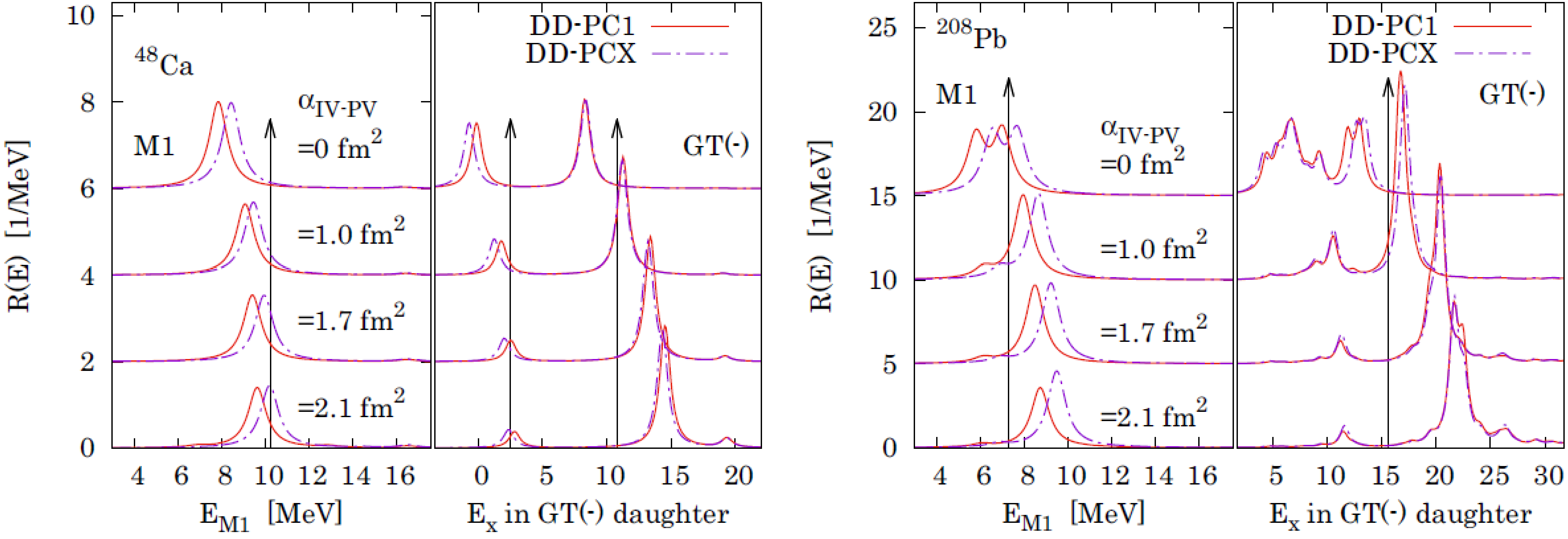
The present REDF somehow does not reproduce the Gamow-Teller and M1 simultaneously…

$$\hat{\mathcal{O}}_{\nu}^{\rm IVM1} = g_s \mu_{\rm N} \sqrt{\frac{3}{4\pi}} \sum_{k \in A} \hat{\tau}_0(k) \hat{s}_{\nu}(k),$$

$$\hat{\mathcal{O}}_{\nu}^{\rm GT(\pm)} = \sum_{k \in A} \hat{\tau}_{\mp}(k) \hat{s}_{\nu}(k),$$

$$\mathcal{L}_{\rm IV-PV} = -\hbar c \frac{\alpha_{\rm IV-PV}}{2} \left[\bar{\psi}\gamma_5 \gamma_{\mu} \vec{\tau} \psi\right] \left[\bar{\psi}\gamma_5 \gamma^{\mu} \vec{\tau} \psi\right]$$

➔ Possibly because we neglect several channels after Fiertz transformation: talk by Q. Zhao this morning.



Summary

- ✓ Relativistic (as well as non-rela') EDF theories are expected to realize the universal, phenomenological model to widely compute the static and dynamic properties of atomic nuclei.
- ✓ M1 excitation: the DD-PC1 + S=0 pairing calculation can approximately reproduce the experimental M1 response. On the other side, the S=1 pairing predicts the low-lying M1 peak, which has not been observed.
- ✓ Future works: (1) how to reproduce the nuclear Gamow-Teller and M1 responses simultaneously; (2) evaluation of proton-emissions with various (R)EDFs; (3) properties of S_{12}=1 pairing mode in atomic nuclei or/and nuclear matter.

OMAKE

NN scat. in many channels

Ryozo Tamagaki, Prog. Theo. Phys. Vol. 44, 905-928 (1970): theoretical evaluation.

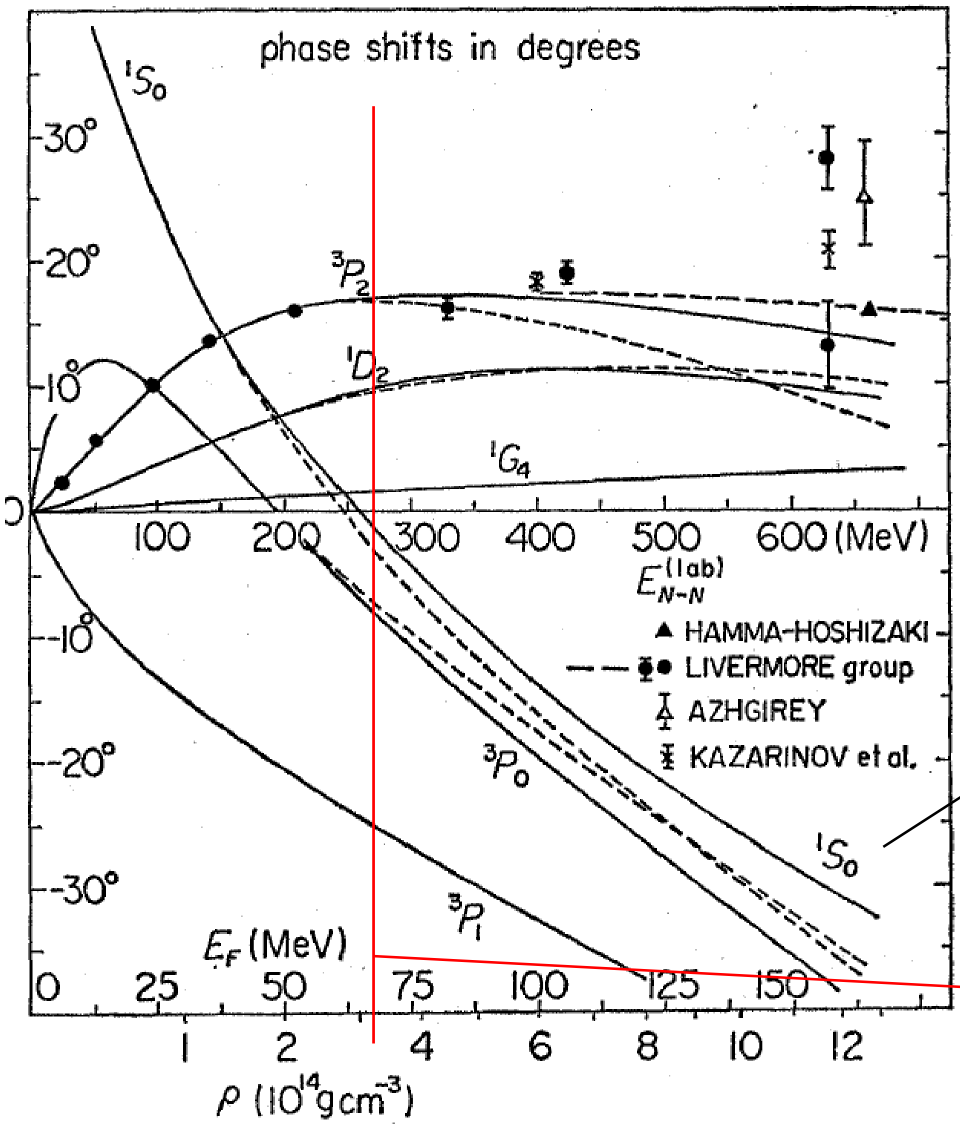
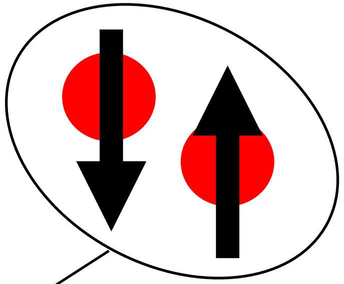


Fig. 1. Nucleon-nucleon scattering phase shifts versus $E_{N\text{-}N}^{(\mathrm{LAB})}=4E_F$. Solid (dotted) lines represent the phase shifts calculated from the OPEG potential with 2 GeV soft core (the OPEH potential with the hard core radius=0.42 fm).[9] For the $^3P_2$ phase shifts, solutions of the phase shift analysis are shown.[10]



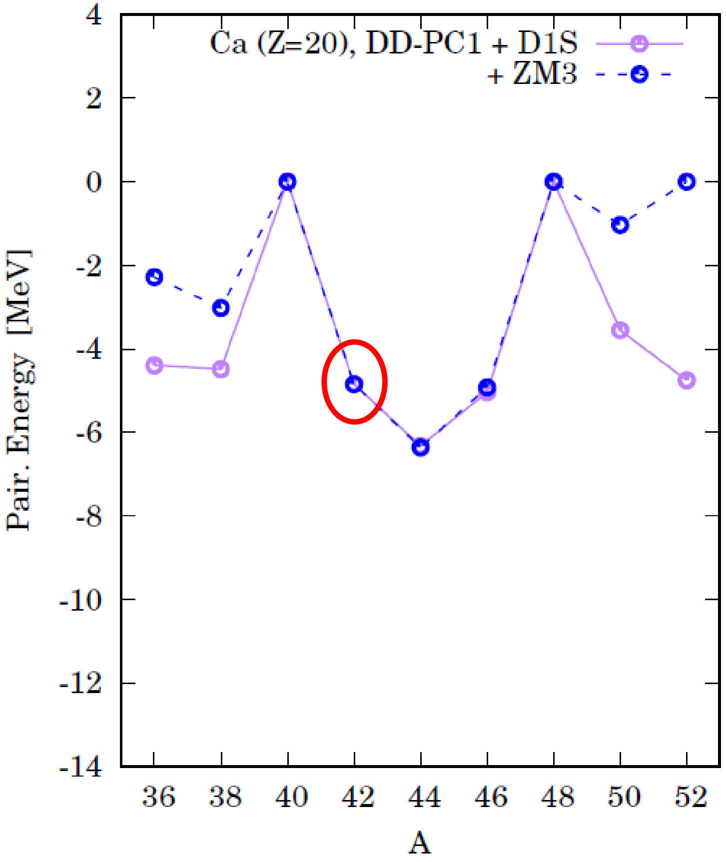
Normal density of nuclear matter:

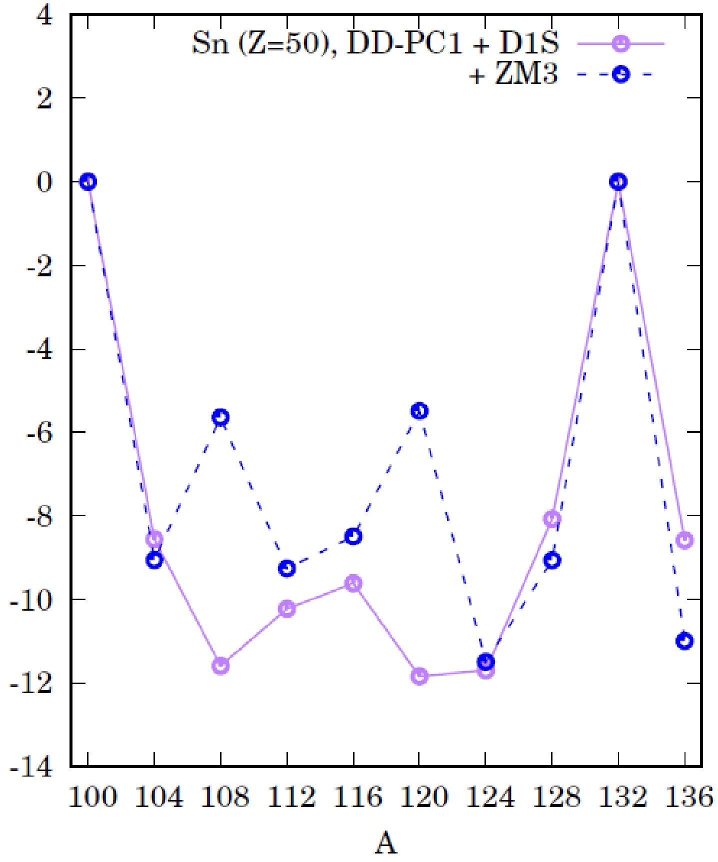
$\rho \cong 3.2\times 10^{14}\,\mathrm{g\,cm^{-3}}$

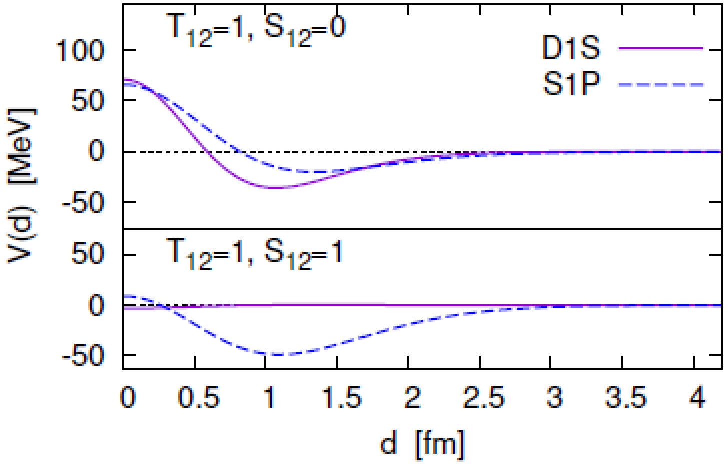
Two pairing models

T.O., G. Kruzic, N. Paar, Eur. Phys. J. A 57, 1-7 (2021) +α.

Two pairing models for S_{12}=0 and S_{12}=1 modes are compared. Those are tuned to equivalently output $\Delta_{pair.}$ = -4.84 MeV for ^{42}Ca.







$$V_{pp} = \sum_{i=a,b} \left\{ (W_i - H_i) + (B_i - M_i)\hat{P}_\sigma \right\} e^{-\frac{d^2}{\mu_i^2}},$$

D1S ➔ S_{12}=0 pairing is dominant.
ZM3 ➔ S_{12}=1 pairing is dominant (S1P).
For several GS solutions, two models show a different gaps.

Quasi-particle random-phase approximation (QRPA)

[0] Hartree-(Fock)-Bogoliubov solves the ground state of quasi-particles. Then the excited states are generally given as follows.

$$\hat{\mathcal{H}} \left|\omega\right\rangle = E_\omega \left|\omega\right\rangle, \quad \left|\omega\right\rangle = \hat{\mathcal{Z}}^\dagger(\omega) \left|\Phi\right\rangle \quad \Longleftrightarrow \quad \left[\hat{\mathcal{H}},\ \hat{\mathcal{Z}}^\dagger(\omega)\right] = \hbar\omega \hat{\mathcal{Z}}^\dagger(\omega), \quad \left[\hat{\mathcal{H}},\ \hat{\mathcal{Z}}(\omega)\right] = -\hbar\omega\hat{\mathcal{Z}}(\omega),$$

$$\hat{\mathcal{W}}(t) \equiv \hat{\mathcal{Z}}^\dagger(\omega)e^{-i\omega t} - \hat{\mathcal{Z}}(\omega)e^{i\omega t}, \quad i\hbar\frac{\partial}{\partial t}\hat{\mathcal{W}}(t) = \left[\hat{\mathcal{H}},\ \hat{\mathcal{W}}(t)\right]$$

[1] QRPA assumption: we only consider the one-body-operator type, where its spin-parity couples to (J, P).

$$\hat{\mathcal{Z}}^\dagger(\omega) = \frac{1}{2}\sum_{\rho\neq\sigma}\left\{X_{\rho\sigma}(\omega)\hat{\mathcal{O}}^{(J,P)\dagger}_{\sigma\rho} - Y^*_{\rho\sigma}(\omega)\hat{\mathcal{O}}^{(J,P)}_{\sigma\rho}\right\}, \quad \text{where } \hat{\mathcal{O}}^{(J,P)}_{\sigma\rho} = \left[a_\sigma \otimes a_\rho\right]^{(J,P)}$$

[2] Amplitudes (X & Y) can be obtained from the matrix QRPA equation.

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix} = \hbar\omega \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} X(\omega) \\ Y^*(\omega) \end{pmatrix},$$

$$A_{ab,cd} \equiv \left\langle \Phi \left[a_b a_a,\ \mathcal{H}a^\dagger_c a^\dagger_d - a^\dagger_c a^\dagger_d \mathcal{H}\right] \Phi \right\rangle, \quad = (E_a + E_b)\delta_{ac}\delta_{bd} + H^{22}_{ab,cd},$$

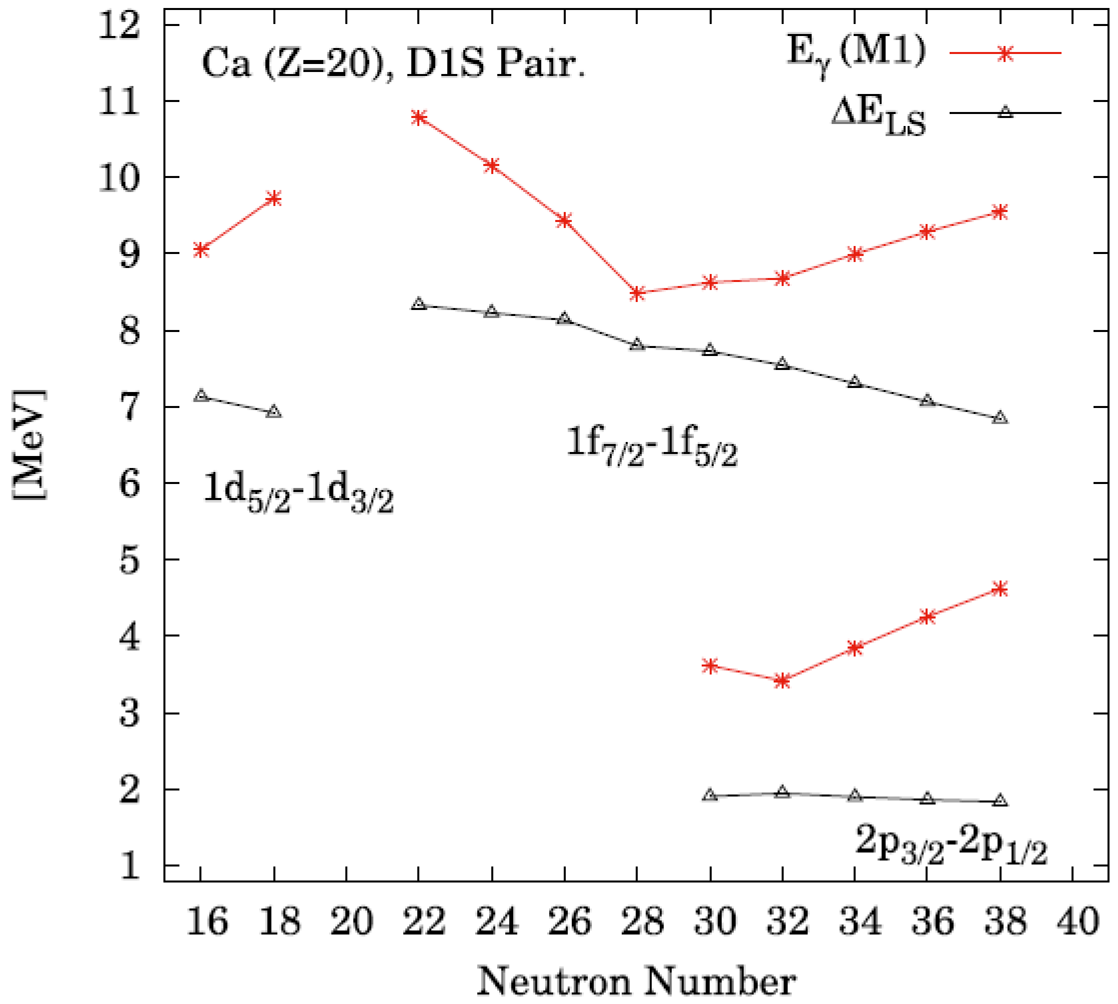
$$B_{ab,cd} \equiv (-)\left\langle \Phi \left[a_b a_a,\ \mathcal{H}a_d a_c - a_d a_c \mathcal{H}\right] \Phi \right\rangle \quad = 4! \cdot H^{40}_{abcd},$$

➔ QRPA matrices A & B are determined from the effective interaction (Lagrangian). Those are numerically calculated and diagonalized.

➔ Note that the numerical cost can be a problem.

LS-splitting gaps v.s. actual M1-excitation energies

T.O., G. Kruzic, N. Paar, J. Phys. G 47, 115106 (2020).



ΔE_{LS} ⇔ RHB ground states.

v.s.

Eγ (M1) ⇔ QRPA-excited states.

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^{(\omega)} \\ Y^{(\omega)} \end{pmatrix} = \hbar\omega \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} X^{(\omega)} \\ Y^{(\omega)} \end{pmatrix}$$

ΔE_{LS} does not coincide exactly with the actual M1 energies.

What does make the difference?

➔ Residual interactions:

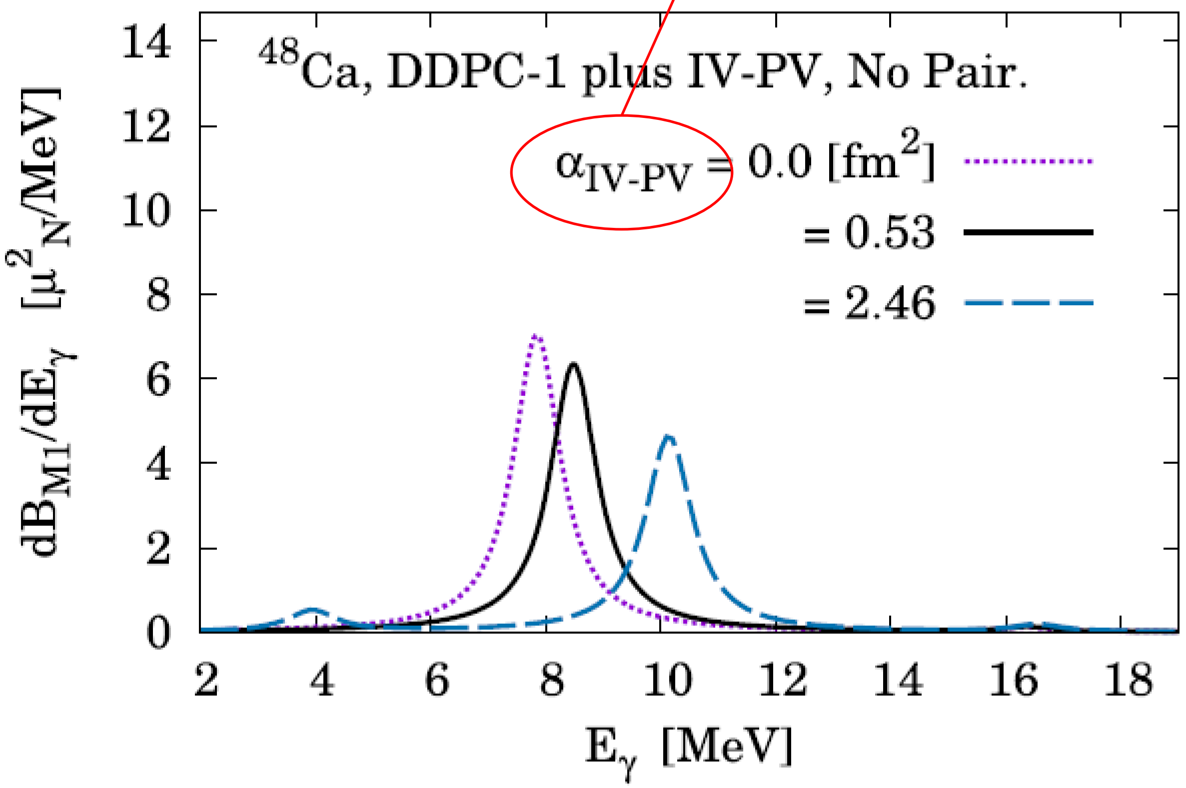
(1) IV-PV in the ph channel;

(2) Pairing in the pp channel.

IV-PV interaction's effect on M1 (^{48}Ca)

$$\frac{dB_{M1}}{dE_\gamma} = \sum_f \delta(E_\gamma - \hbar\omega_f) \sum_\nu \left| \left\langle \omega_f \middle| \hat{Q}_\nu(\mathrm{M1}) \middle| \Phi \right\rangle \right|^2,$$ with

$$\mathcal{L}_{\mathrm{IV-PV}} = -\hbar c \frac{\alpha_{\mathrm{IV-PV}}}{2} \left[\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi\right] \left[\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi\right]$$

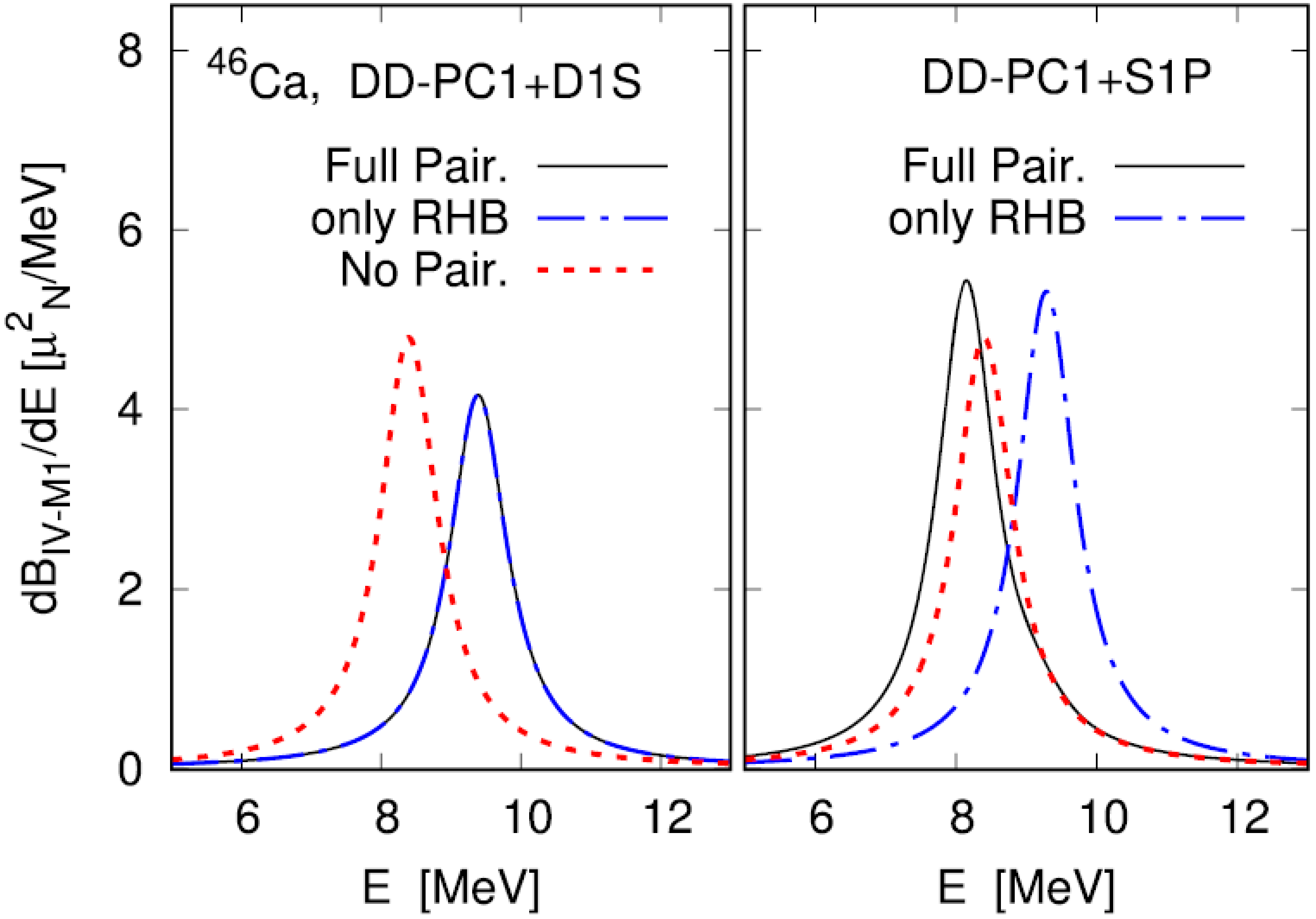


(1) DD-PC1 for ph-RHB;
(2) IV-PV (residual int.) for ph-QRPA.
(3) Pairing vanishes for ^{48}Ca.
➔ The IV-PV residual interaction noticeably affects the M1-transition energy.

Note: in the GS (0+) solutions from the RHB, the IV-PV does not make a finite effect.

S=0/1 pairing in QRPA

T.O., G. Kruzic, N. Paar, J. Phys. G 47, The European Physical Journal A, Vol. 57(6), page 1-7 (2021).



Pairing potentials is switched off in the RHB/QRPA calculations.

➔ S_{12}=1 pairing (S1P=ZM3) model provides an additional attractive force for the M1-excited states.

➔ S_{12}=0 pairing (D1S) model cannot affect the excited states.

Method:

(i) REDEF-based Hartree-Bogoliubov

(ii) quasi-particle random-phase approximation (QRPA)

Milestones of nuclear EDF theory

Hohenberg-Kohn theorem (multi-electron systems) *Phys. Rev. 136, B844 (1964).*
Ground state Φ as well as its energy are functionals of the density $\rho(x) = \langle\Phi|\psi^+(x)\psi(x)|\Phi\rangle$. Once the EDF, $\mathrm{E}[\rho(x)] = \langle\Phi[\rho]|\hat{H}|\Phi[\rho]\rangle$ is found, the ground state can be solved by the density-variational principle.

Kohn-Sham method (multi-electron systems) *Phys. Rev. 140, A1133 (1965).*
Implementation of the density-variational principle is shown as applicable.

EDF theory for multi-nucleon systems

- (1970~) Phenomenological self-consistent meanfield calculations with Skyrme, Gogny, Rela' point-coupling, etc. E.g. *D. Vautherin and D. M. Brink, Phys. Rev. C 5, 626 (1972).*
- (2000~) Those meanfield calculations are re-considered as the products of nuclear EDF theory.

Point-Coupling REDF Lagrangian

In the relativistic nuclear theory (RNT), nucleon is described by a Dirac spinor $\psi(x)$, where $x = \{\boldsymbol{r}, \boldsymbol{s}, \vec{\tau}\}$. The phenomenological Lagrangian density reads

$$\mathcal{L} = \bar{\psi}(x)[i\gamma_\mu \partial^\mu - M]\psi(x) + \mathcal{L}_{\mathrm{M}} + \mathcal{L}_{\mathrm{I}}. \quad (1)$$

TABLE 2: Interaction terms included in $\mathcal{L}_{\mathrm{I}}$. Label (i) indicates isoscalar (IS) or isovector (IV). Label (ii) indicates scalar (S), vector (V), pseudo-scalar (PS) or pseudo-vector (PV).

(i)	(ii)	(T, J^π)	Meson	Meson-exchange	Point-coupling
IS	S	$(0, 0^+)$	σ	$-g_\sigma \bar{\psi}\sigma\psi$	$-\alpha_{\mathrm{IS-S}}(\rho)[\bar{\psi}\psi][\bar{\psi}\psi]/2$
					$-\delta_{\mathrm{IS-S}}(\rho)\partial_\mu[\bar{\psi}\psi]\partial^\mu[\bar{\psi}\psi]/2$
	V	$(0, 1^-)$	ω^μ	$-g_\omega[\bar{\psi}\gamma_\mu\omega^\mu\psi]$	$-\alpha_{\mathrm{IS-V}}(\rho)[\bar{\psi}\gamma_\mu\psi][\bar{\psi}\gamma^\mu\psi]/2$
	PS	$(0, 0^-)$	$\times$	$\times$	$\times$
	PV	$(0, 1^+)$	$\times$	$\times$	$\times$
IV	S	$(1, 0^+)$	$\times$	$\times$	$\times$
	V	$(1, 1^-)$	$\vec{\rho}^\mu$	$-g_\rho[\bar{\psi}\gamma_\mu(\vec{\tau}\vec{\rho}^\mu)\psi]$	$-\alpha_{\mathrm{IV-V}}(\rho)[\bar{\psi}\gamma_\mu\vec{\tau}\psi][\bar{\psi}\gamma^\mu\vec{\tau}\psi]/2$
	PS	$(1, 0^-)$	$\vec{\pi}$	$-ig_\pi[\bar{\psi}\gamma_5(\vec{\tau}\vec{\pi})\psi]$	$-\alpha_{\mathrm{IV-PS}}(\rho)[\bar{\psi}\gamma_5\vec{\tau}\psi][\bar{\psi}\gamma_5\vec{\tau}\psi]/2$
	PV	$(1, 1^+)$	$\partial_\mu\vec{\pi}$	$-\frac{f_\pi}{m_\pi}[\bar{\psi}\gamma_5\gamma_\mu\partial^\mu(\vec{\tau}\vec{\pi})\psi]$	$-\alpha_{\mathrm{IV-PV}}(\rho)[\bar{\psi}\gamma_5\gamma_\mu\vec{\tau}\psi][\bar{\psi}\gamma_5\gamma^\mu\vec{\tau}\psi]/2$
Coulomb					$-e\bar{\psi}\gamma_\mu A^\mu\left(\frac{1-\hat{\tau}_3}{2}\right)\psi$

In this work, we employ the point-coupling model.

Setting = DD-PC1 parameters.

References:

[1] T. Niksic, D. Vretenar, and P. Ring, Progress in Particle and Nuclear Physics 66(3), 519-548 (2011). [2] T. Niksic et. al., Comp. Phys. Communications, 107184 (2020).

Relativistic Hartree method

※Fock term is neglected, and DD-PC1 parameters are re-optimized.

For example, DD-PC1 Lagrangian ➔ DD-PC1 Hamiltonian. $\mathcal{H}(x) \equiv (\partial_0 \psi^\dagger) \frac{\delta \mathcal{L}}{\delta (\partial_0 \psi^\dagger)} + \frac{\delta \mathcal{L}}{\delta (\partial_0 \psi)} (\partial_0 \psi) - \mathcal{L}$

(1) We assume the relativistic Hartree ground-state solution as single-Slater determinant of the particle-basis states.

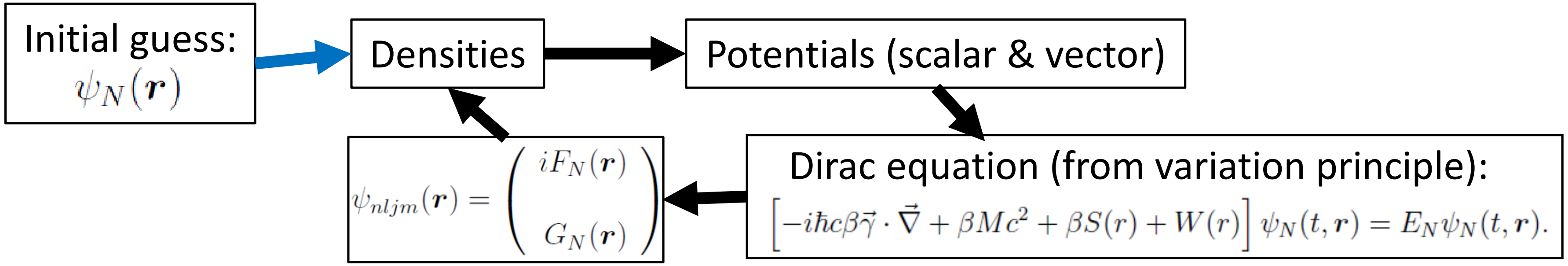
$$|\mathrm{HF}\rangle = c_A^\dagger \cdots c_1^\dagger \left|-\right\rangle.$$

Then, the Hamiltonian is also formally represented within these basis:

$$H(t) = \sum_{r,s} \int dE' \int dE \int d^3\boldsymbol{r}$$

$$\left[u_{r,E'}^\dagger(x) c_{r,E'}^\dagger + v_{r,-E'}^\dagger(x) b_{r,-E'}^\dagger \right] \hat{h}_D \left[u_{s,E}(x) c_{s,E} + v_{s,-E}(x) b_{s,-E} \right]$$

(2) No-sea approximation: we neglect the Dirac-sea states with negative energies.
(3) The particle states are obtained from the self-consistent mean-field Dirac equation:



Bogoliubov transformation

$c_k^\dagger$ & $c_k \cdots$ Original creation & annihilation,
$a_k^\dagger$ & $a_k \cdots$ QP creation & annihilation.

Hamiltonian in the true-particle representation:

$$\hat{\mathcal{H}} = \sum_{kl} \epsilon_{kl} c_k^\dagger c_l + \frac{1}{4} \sum_{a \neq b} \sum_{c \neq d} \tilde{v}_{ab,cd} \left(c_b c_a \right)^\dagger c_d c_c,$$

(1) Before the Bogoliubov transformation = pairing correlation, the HF-ground state is obtained as single-Slater determinant of the true-particle states.

$$|\mathrm{HF}\rangle = c_A^\dagger \cdots c_1^\dagger |-\rangle.$$

(2) Then we move to the HFB-ground state by the Bogpoliubov transformation.

$$\begin{pmatrix} a_\downarrow \\ a_\downarrow^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix} \equiv \hat{\mathcal{W}}^\dagger \begin{pmatrix} c_\downarrow \\ c_\downarrow^\dagger \end{pmatrix}$$

These Bogoluibov coefficients (U & V) are determined so as to minimize the <H> including the pairing gap.
How to solve them numerically? ➔ H(F)B equation.

$$\sum_l \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}_{kl} \begin{pmatrix} U_{lm} \\ V_{lm} \end{pmatrix} = \delta_{km} E_m \begin{pmatrix} U_{km} \\ V_{km} \end{pmatrix}.$$

$$h_{kl} = \epsilon_{kl} + \Gamma_{kl}, \quad \Gamma_{kl} = \sum_{pq} \tilde{v}_{kq,lp} \rho_{pq},$$

$$\Delta_{kl} = \frac{1}{2} \sum_{pq} \tilde{v}_{kl,pq} \kappa_{pq}.$$

$$\rho_{kl} \equiv \left\langle \Phi \mid c_l^\dagger c_k \mid \Phi \right\rangle,$$

$$\kappa_{kl} \equiv \langle \Phi \mid c_l c_k \mid \Phi \rangle,$$

Quasi-particle random-phase approximation (QRPA)

[0] Hartree-(Fock)-Bogoliubov solves the ground state of quasi-particles. Then the excited states are generally given as follows.

$$\hat{\mathcal{H}}\left|\omega\right\rangle = E_\omega \left|\omega\right\rangle, \quad \left|\omega\right\rangle = \hat{\mathcal{Z}}^\dagger(\omega)\left|\Phi\right\rangle \quad \Leftrightarrow \quad \left[\hat{\mathcal{H}},\ \hat{\mathcal{Z}}^\dagger(\omega)\right] = \hbar\omega\hat{\mathcal{Z}}^\dagger(\omega), \quad \left[\hat{\mathcal{H}},\ \hat{\mathcal{Z}}(\omega)\right] = -\hbar\omega\hat{\mathcal{Z}}(\omega),$$

$$\hat{\mathcal{W}}(t) \equiv \hat{\mathcal{Z}}^\dagger(\omega)e^{-i\omega t} - \hat{\mathcal{Z}}(\omega)e^{i\omega t}, \quad i\hbar\frac{\partial}{\partial t}\hat{\mathcal{W}}(t) = \left[\hat{\mathcal{H}},\ \hat{\mathcal{W}}(t)\right]$$

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$$B_{ab,cd} \equiv (-)\left\langle\Phi\left[a_b a_a,\ \mathcal{H}a_d a_c - a_d a_c \mathcal{H}\right]\Phi\right\rangle = 4!\cdot H^{40}_{abcd},$$

➔ QRPA matrices A & B are determined from the effective interaction (Lagrangian). Those are numerically calculated and diagonalized.

➔ Note that the numerical cost can be a problem.

What "relativistic" EDF provides?

Relativistic EDF (Covariant DF) Theory
= effective field theory of nucleons and mesons.

$$\begin{aligned} \mathcal{L}_{\rm REDF} &= \bar{\psi}(x)\left[i\,\partial\!\!\!/ - m\right]\psi(x) \\ &\quad +\mathcal{L}_{\rm meson} + \mathcal{L}_{\rm int}, \quad \text{where} \\ \psi(x) &\cdots \text{nucleon,} \\ \mathcal{L}_{\rm meson} &\cdots \text{free mesons,} \\ \mathcal{L}_{\rm int} &\cdots \text{interactions.} \end{aligned}$$

Motivation & Caution to choose the REDF framework:

- ✓ In the original work by J.D. Walecka [1], his original motivation was to obtain the stress tensor for the Einstein equation of neutron stars. This purpose needs the relativistic formalism. As a successful result by Walecka [1], the repulsive core of the nuclear force in the high-density region can be naturally concluded.
- ✓ The Dirac-Lorentz formalism leads to a consistent treatment of spin degrees of freedom as well as an unified description of time-even and time-odd fields [2]. Also, the relativistic effect and causality can be included [1-4].
- ✓ Connection between the force and meson is clear: e.g. tensor force is from one-pion exchange (pseudo-scalar & pseudo-vector coupling) [4].
- ✓ Spin-orbit (LS) level splitting, which is one fundamental feature of atomic nuclei, is naturally concluded [2-4]. This character could be a key to evaluate e.g. the charge distribution, M1 and Gamow-Teller excitations, etc.

References: [1] J. D. Walecka, Ann. of Phys. 83, 491 (1974); [2] D. Vretenar et al., Phys. Report 409, 101-259 (2005); [3] P.-G. Reinhard, Rep. on Progress in Phys. 52, 439 (1989); [4] 土岐博＆保坂淳、「相対論的多体系としての原子核」、大阪大学出版会(2011).

Spin-orbit (LS) splitting from Dirac eq.

$$\left[-i\hbar c\beta\vec{\gamma}\cdot\vec{\nabla}+\beta Mc^2+\beta S(r)+W(r)\right]\psi_N(t,\boldsymbol{r})=E_N\psi_N(t,\boldsymbol{r}).$$

Scalar meson(s)

Vector meson(s)

$$\psi_N(\boldsymbol{r})=\psi_{nljm}(\boldsymbol{r})=\begin{pmatrix} iF_N(\boldsymbol{r}) \\ G_N(\boldsymbol{r})\end{pmatrix}=\begin{pmatrix} if_{nlj}(r)\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \\ g_{nlj}(r)\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}})\end{pmatrix}$$

$$\left[-\frac{(\hbar c)^2}{\epsilon_N(r)}\nabla^2-(\hbar c)^2\frac{(-)\epsilon'_N(r)}{\epsilon_N^2(r)}\frac{d}{dr}+\frac{(\hbar c)^2}{r}\frac{(-)\epsilon'_N(r)}{\epsilon_N^2(r)}\frac{2\vec{S}\cdot\vec{L}}{\hbar^2}\right.$$
$$\left.+S(r)+W(r)\right]F_N(\boldsymbol{r}) = (E_N-Mc^2)F_N(\boldsymbol{r}),$$

where the 1st term in the LHS corresponds to the kinetic energy, the 2nd term is so-called Darwin term, and the 3rd term indicates the spin-orbit coupling. These Darwin and spin-orbit terms can be naturally concluded from the Dirac equation, whereas those were just introduced as "phenomenology" in the Schroedinger equation.

It is convenient to find that,

- the total potential is given as $S(r)+W(r)$, whereas,
- the spin-orbit and Darwin terms depend on the $\epsilon'_N(r)=S'(r)-W'(r)$.

My channel in YouTube

https://www.youtube.com/playlist?list=PLRxfmYDVpOKjTWNCDV-y8965BoncZ_5fP