



半微視的汎関数による Kohn-Sham 型理論の 核子・原子核散乱への拡張的応用

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@ 京大益川ホール (Feb. 16 – 18, 2026)

H.N. & K. Ishida, PRC 109, 044614; 110, 019901(E)
K. Ishida & H.N., PRC 111, 044610

Before starting ...

The 5th Conference on Advances in Radioactive Isotope Science



ARIS 2026

Advances in Radioactive Isotope Science
FUKUSHIMA, JAPAN

June 1-7 | Iizaka Onsen
May 31: Public Lecture | Palthe Iizaka

Scope

- Nuclear structures
- Nuclear reactions and responses
- Nuclear equation of state
- Nuclei at and beyond the drip lines
- Heaviest elements and fission
- Nuclear forces and a few-body physics
- Nuclear astrophysics, nucleosynthesis
- Fundamental symmetries and interactions
- New approaches in nuclear theory
- New instruments and methods in experiments
- Radioactive ion beam productions and new isotope searches
- Nuclear science for society

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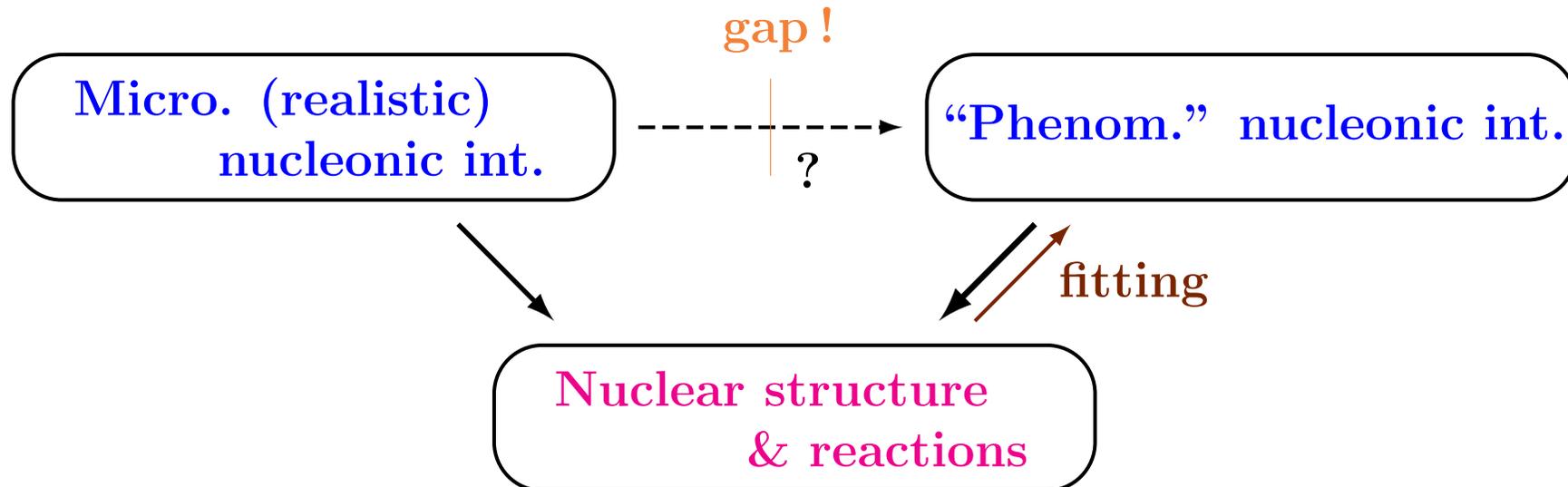
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I. Introduction

★ Nuclear properties & nucleonic interaction



“gap” b/w micro. int. & phenom. int. (in KS / SCMF approach)
 — needs to be filled!

- **micro. int.** → precision for E/A : a few 100 keV $\approx 2\%$
vs. KS w/ phenom. int.

→ precision for ^{208}Pb : a few MeV out of 1.6 GeV $\approx 0.2\%$

- **phenom. int.** (\leftarrow fitting)

→ not extendable to unfitted quantities

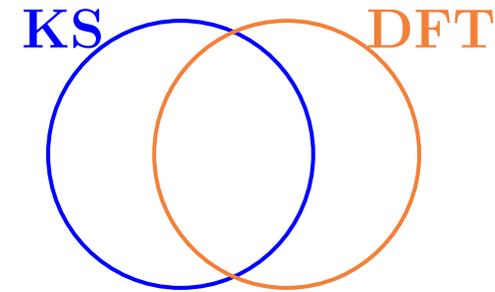
⇒ **KS approach** w/ “**semi-realistic int.**” (\dots fine tuning)

★ “Minimal composition” (\approx “essence”) of Kohn-Sham theory

H.N., Phys. Scr. 98, 105007

$$E^{\text{KS}}[\rho] \leftarrow E[Q[\rho]] = \min_{\Psi \rightarrow Q} E[\Psi]$$

Q : principal variables
 ($n(\mathbf{r}) \in Q \dots$ unnecessary!)
 ρ : 1-b. DM



★ “ v -representability” = differentiability \leftrightarrow universality of $E^{\text{KS}}[\rho]$
 — should not be disregarded!

★ KS orbitals \dots artifact? \rightarrow “quasiparticle” à la Landau
 (= dressed particle)

$$|\Psi^{\text{exact}}\rangle = \mathcal{U}(0, -\infty) |\Phi^{\text{KS}}\rangle \quad \mathcal{U}(t, t_0): \text{time-evolution op.}$$

$$(H \rightarrow h^{\text{KS}} + (H - h^{\text{KS}}) e^{\eta t})$$

\therefore) adiabatic theorem

$$= \mathcal{U}(0, -\infty) \left[\prod_{i=1}^N a_i^{\text{KS}\dagger} |0\rangle \right] = \prod_{i=1}^N \underbrace{[\mathcal{U}(0, -\infty) a_i^{\text{KS}\dagger} \mathcal{U}^{-1}(0, -\infty)]}_{\text{“quasiparticle”}} |0\rangle$$

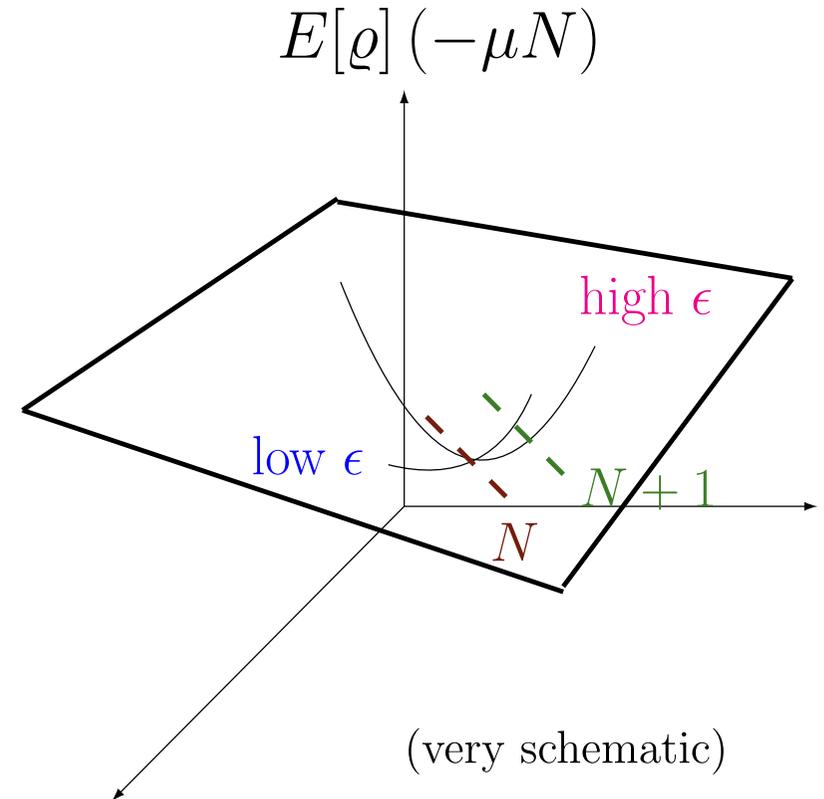
★ Extension of KS approach to s.p. states at $\epsilon > 0$

structure of $E^{\text{KS}}[\rho]$? (— complicated manifold)

$$h^{\text{KS}} = \frac{\delta E^{\text{KS}}}{\delta \rho} = \frac{p^2}{2M} + \underset{\uparrow}{U^{\text{KS}}} \rightarrow \text{s.p. states}$$

containing many-body corr.

- minimization
 - ↔ small-“curvature” submanifold
 - ↔ low- ϵ s.p. states
- high- ϵ s.p. states (incl. $\epsilon > 0$)
 - ↔ large-“curvature” submanifold
- v -representability (for g.s.)
 - ↔ universality w.r.t. particle #?



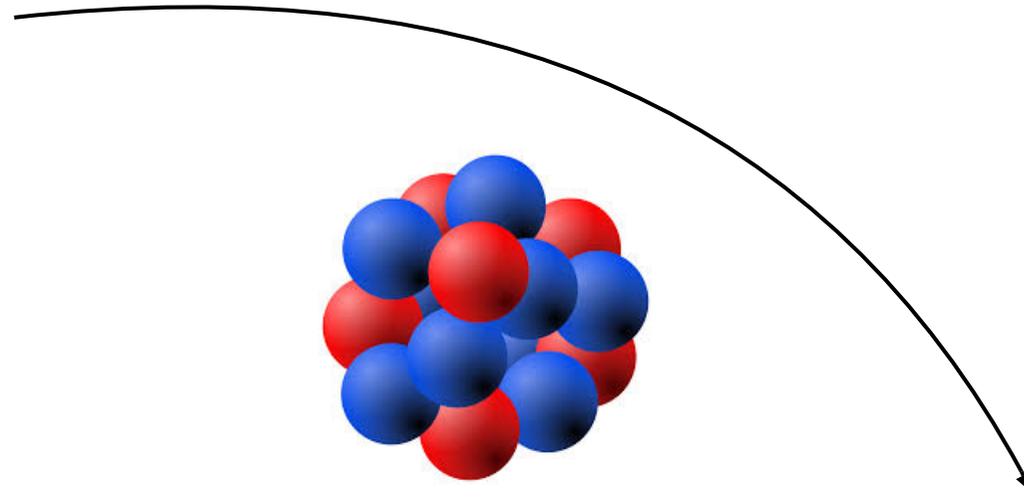
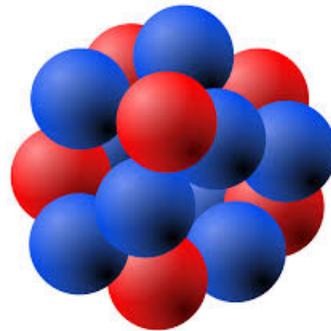
U^{KS} at $\epsilon > 0$ ↔ real part of optical pot. ν^{SFP}
 many-body corr. ↔ “dynamical pol. effect”
 imag. part? — beyond MF (KS)

cf. $\delta^2 E / \delta \rho^2$ ↔ RPA or TDKS

★ N - A scattering

$$|\Psi_A\rangle \otimes |\psi_N\rangle \rightarrow \left\{ \begin{array}{l} |\Psi_A\rangle \otimes |\psi_N\rangle \quad (\text{elastic}) \\ |\Psi_A^*\rangle \otimes |\psi_N\rangle \quad (\text{inelastic}) \\ |\Psi_{A_1}\rangle \otimes |\Psi_{A_2}\rangle \\ \vdots \end{array} \right\} \rightarrow \text{“absorption”}$$

channel branching — beyond KS



“KS approach” to elastic channel: $E^{\text{KS}}[\rho] \rightarrow \left\{ \begin{array}{l} |\Psi_A\rangle \approx |\Phi_A^{\text{KS}}\rangle \\ (\nu^{\text{SFP}} \rightarrow) |\psi_N\rangle \\ \text{“dressed nucleon”} \end{array} \right.$

II. Self-consistent single-nucleon potential

★ Self-consistent pot. from eff. int. (or EF) ⇐ variational principle

$$E[\varrho] = \sum_{\alpha\alpha'} \langle \alpha | \frac{\mathbf{p}^2}{2M} | \alpha' \rangle \varrho_{\alpha'\alpha} + \frac{1}{2} \sum_{\alpha\alpha'\beta\beta'} \langle \alpha\beta | \hat{v}_{\text{eff}} | \alpha'\beta' \rangle \varrho_{\alpha'\alpha} \varrho_{\beta'\beta}$$

$$\rightarrow h|\alpha^{(0)}\rangle = \epsilon_{\alpha^{(0)}}|\alpha^{(0)}\rangle \quad \text{with} \quad h = \sum_{\alpha\alpha'} |\alpha\rangle \frac{\delta E}{\delta \varrho_{\alpha'\alpha}} \Big|_{\varrho^{(0)}} \langle \alpha'| = \frac{\mathbf{p}^2}{2M} + U$$

input: **eff. int.** (or **EF**) $\dots \hat{v}_{\text{eff}} = \sum_i C_i[n(\mathbf{r})] \cdot \hat{w}_i$

\hat{w}_i : two-body operator

$$\begin{aligned} \rightarrow U|\alpha\rangle &= \sum_i \sum_{\beta\beta'} \langle * \beta | C_i[n^{(0)}(\mathbf{R}_{\alpha\beta})] \cdot \hat{w}_i | \alpha\beta' \rangle \varrho_{\beta\beta'}^{(0)} \\ &+ \frac{1}{2} |\alpha\rangle \sum_i \sum_{\alpha''\alpha'\beta\beta'} C_i[n^{(0)}(\mathbf{r}_\alpha)] \langle \alpha''\beta | \delta(\mathbf{r}_\alpha - \mathbf{R}_{\alpha''\beta}) \cdot \hat{w}_i | \alpha'\beta' \rangle \varrho_{\alpha'\alpha''}^{(0)} \varrho_{\beta'\beta}^{(0)} \end{aligned}$$

↑
rearrangement term

$$\begin{cases} \min E_A[\varrho^{(0)}] \text{ (iterative)} & \rightarrow |\Phi_A\rangle \\ U (= \mathcal{V}^{\text{SFP}}) \text{ from } E_{A+1}[\varrho^{(0)} + \delta\varrho] & \rightarrow |\psi_N\rangle \quad (\varrho^{(0)} \leftrightarrow |\Phi_A\rangle) \end{cases}$$

★ Finite-range eff. int. (\leftrightarrow non-local EF)

— possibly important to cover high ϵ

- SCMF code: [MFGSB](#) → accessible @ Chiba U. Repository

(<https://opac.ll.chiba-u.jp/da/curator/900123722/?lang=1>; DOI: 10.20776/900123722)

- GEM (multi-range Gaussian bases)
- adapted to finite-range int. \dots **Yukawa f.f.** (& tensor force)
- able to describe halo
- complete formulae for $U^{\text{KS}} (= \mathcal{V}^{\text{SFP}})$ → derived (up to $\hat{v}_{ij}^{(\text{LS})}$ & $\hat{v}_{ij}^{(\text{TN})}$)
H.N. & K. Ishida, PRC 109, 044614
- new code applicable to non-local optical pot. → available
(e.g. [SIDES](#))

exchange term
of $\hat{v}_{ij}^{(\text{LS})}$:

$$\begin{aligned}
F_{\ell j, \tau_\alpha}^{(\text{exc, LS})} \mathcal{R}_{\ell j}(r) &= \frac{1}{2} \sum_{\substack{\ell_\alpha j_\alpha \\ \nu_\alpha \nu_{\alpha'} \in A}} (2\ell_\alpha + 1)(2j_\alpha + 1) \varrho_{\nu_\alpha \nu_{\alpha'}}^{(\tau_\alpha \ell_\alpha j_\alpha)} \sum_{\lambda} (2\lambda + 1) (\ell_\alpha 0 \lambda 0 | \ell 0)^2 \begin{Bmatrix} \ell_\alpha & 1/2 & j_\alpha \\ \lambda & 0 & \lambda \\ \ell & 1/2 & j \end{Bmatrix}^2 \\
&\times \left\{ j(j+1) - \ell(\ell+1) - \frac{3}{4} + j_\alpha(j_\alpha+1) - \ell_\alpha(\ell_\alpha+1) - \frac{3}{4} \right\} \\
&\times \int r'^2 dr' g_\lambda(r, r') R_{\nu_{\alpha'} \ell_\alpha j_\alpha}^*(r') R_{\nu_\alpha \ell_\alpha j_\alpha}(r) \mathcal{R}_{\ell j}(r') \\
&+ \sum_{\substack{\ell_\alpha j_\alpha \\ \nu_\alpha \nu_{\alpha'} \in A}} (2\ell_\alpha + 1)(2j_\alpha + 1) \varrho_{\nu_\alpha \nu_{\alpha'}}^{(\tau_\alpha \ell_\alpha j_\alpha)} \\
&\times \sum_{\lambda \lambda' \lambda'' \lambda'''} (2\kappa + 1) (\ell_\alpha 0 \lambda'' 0 | \ell 0) (\ell_\alpha 0 \lambda''' 0 | \ell 0) \begin{Bmatrix} \ell_\alpha & 1/2 & j_\alpha \\ \kappa & 0 & \kappa \\ \ell & 1/2 & j \end{Bmatrix} \begin{Bmatrix} \ell_\alpha & 1/2 & j_\alpha \\ \lambda' & 1 & \kappa \\ \ell & 1/2 & j \end{Bmatrix} \\
&\times \int r'^2 dr' g_\lambda(r, r') R_{\nu_{\alpha'} \ell_\alpha j_\alpha}^*(r') \left[\frac{\sqrt{3}}{2} \sqrt{\ell(\ell+1)(2\ell+1)} (\sqrt{2\kappa+1} \delta_{\lambda \lambda'} \delta_{\lambda \lambda''} \delta_{\lambda \lambda'''} W(\ell 1 \ell_\alpha \lambda; \ell \kappa) \right. \\
&- \frac{6r}{r'} \sqrt{(2\lambda'+1)(2\lambda''+1)} (\lambda 0 1 0 | \lambda'' 0) (\lambda 0 1 0 | \lambda''' 0) W(\lambda 1 \kappa 1; \lambda' 1) \\
&\times \{\sqrt{2\kappa+1} \delta_{\lambda' \lambda'''} W(\ell 1 \ell_\alpha \lambda''; \ell \kappa) W(\lambda 1 \kappa 1; \lambda'' 1) \\
&+ \sqrt{2\lambda'+1} \delta_{\kappa \lambda'''} W(\ell 1 \ell_\alpha \lambda''; \ell \lambda') W(\lambda 1 \lambda' 1; \lambda'' 1)\} \left. R_{\nu_\alpha \ell_\alpha j_\alpha}(r) \mathcal{R}_{\ell j}(r') \right. \\
&- (-)^{\lambda'+\kappa} \frac{\sqrt{3}}{2} \sqrt{l_\alpha(l_\alpha+1)(2l_\alpha+1)} (\sqrt{2\kappa+1} \delta_{\lambda \lambda'} \delta_{\lambda \lambda''} \delta_{\lambda \lambda'''} W(\ell_\alpha 1 \ell \lambda; \ell_\alpha \kappa) \\
&- \frac{6r'}{r} \sqrt{(2\lambda'+1)(2\lambda''+1)} (\lambda 0 1 0 | \lambda'' 0) (\lambda 0 1 0 | \lambda''' 0) W(\lambda 1 \kappa 1; \lambda' 1) \\
&\times \{\sqrt{2\kappa+1} \delta_{\lambda' \lambda'''} W(\ell_\alpha 1 \ell \lambda''; \ell_\alpha \kappa) W(\lambda 1 \kappa 1; \lambda'' 1) \\
&+ \sqrt{2\lambda'+1} \delta_{\kappa \lambda'''} W(\ell_\alpha 1 \ell \lambda''; \ell_\alpha \lambda') W(\lambda 1 \lambda' 1; \lambda'' 1)\} \left. R_{\nu_\alpha \ell_\alpha j_\alpha}(r) \mathcal{R}_{\ell j}(r') \right) \\
&- 3\sqrt{2(2\lambda'+1)} \delta_{\kappa \lambda''} \delta_{\lambda' \lambda'''} (\lambda 0 1 0 | \lambda'' 0) (\lambda 0 1 0 | \lambda''' 0) W(\lambda 1 \kappa 1; \lambda' 1) \\
&\times \left. \left\{ r R_{\nu_\alpha \ell_\alpha j_\alpha}(r) \frac{d\mathcal{R}_{\ell j}(r')}{dr'} - (-)^{\lambda'+\kappa} r' \frac{dR_{\nu_\alpha \ell_\alpha j_\alpha}(r)}{dr} \mathcal{R}_{\ell j}(r') \right\} \right]. \tag{B14}
\end{aligned}$$

★ **Eff. int.** (or **EF**) to be used $\dots \hat{v}_{ij} = \hat{v}_{ij}^{(C)} + \hat{v}_{ij}^{(LS)} + \hat{v}_{ij}^{(TN)} + \hat{v}_{ij}^{(C\rho)}$

M3Y int. \dots Yukawa f.f. \rightarrow fit to G -matrix (@ $n \approx n_0/3$)

‘**M3Y-P_n**’

H.N., PRC 68, 014316

- modifying M3Y-Paris $\left\{ \begin{array}{l} \text{replace short-range part of } \hat{v}^{(C)} \text{ by } \hat{v}^{(C\rho)} \\ \text{enhance } \hat{v}^{(LS)} \quad (\leftrightarrow \text{ } l s \text{ splitting}) \end{array} \right.$
- keeping $\hat{v}_{\text{OPEP}}^{(C)}$ (longest-range part)
- no change for $\hat{v}^{(TN)}$ from M3Y-Paris — realistic tensor force

M3Y-P6 : H.N., PRC 87, 014336; IJMPE 29, 1930008

\dots “**semi-realistic**” int. — compromise of micro. & phenom. int.
or “**fine tuning**” of micro. int.

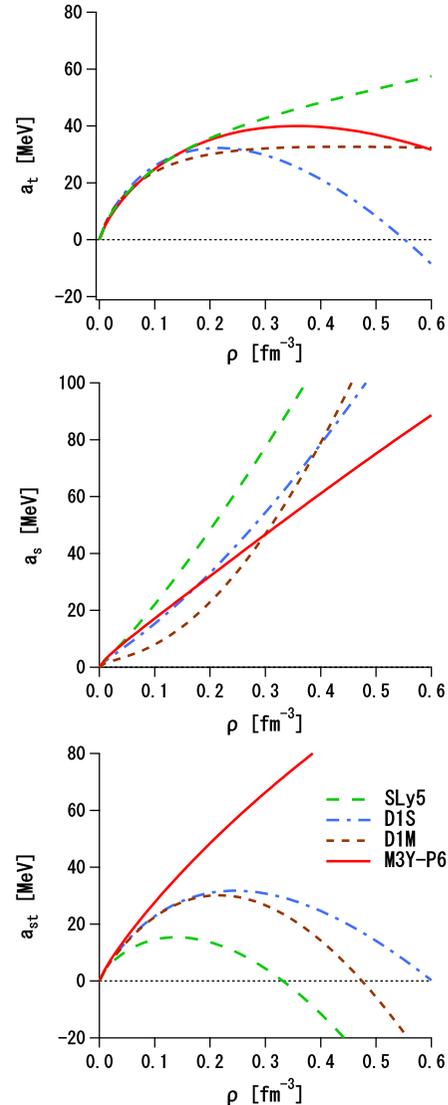
(\dots **attempt to fill the gap!**)

(**Gogny-D1S** & **Skyrme-SLy4** \dots for comparison)

★ **Unphysical instabilities** (— in many SCMF int. even at MF level?)

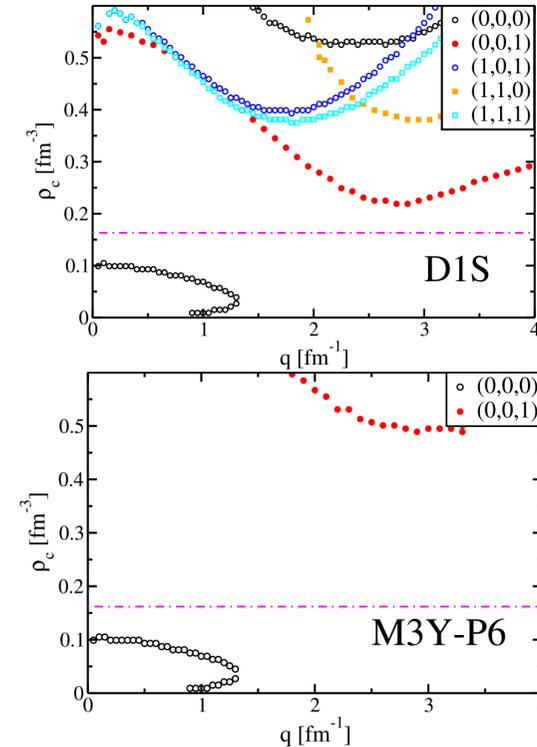
Curvatures of E/A

against spin & isospin exc.:



Instabilities in nuclear matter —

e.g. response fn. (with $\hat{v}^{(\text{TN})}$):



“A quite remarkable result is that the Nakada’s interactions are essentially free from instabilities up to $\approx 2\rho_0$ ”

D. Davesne *et al.*,

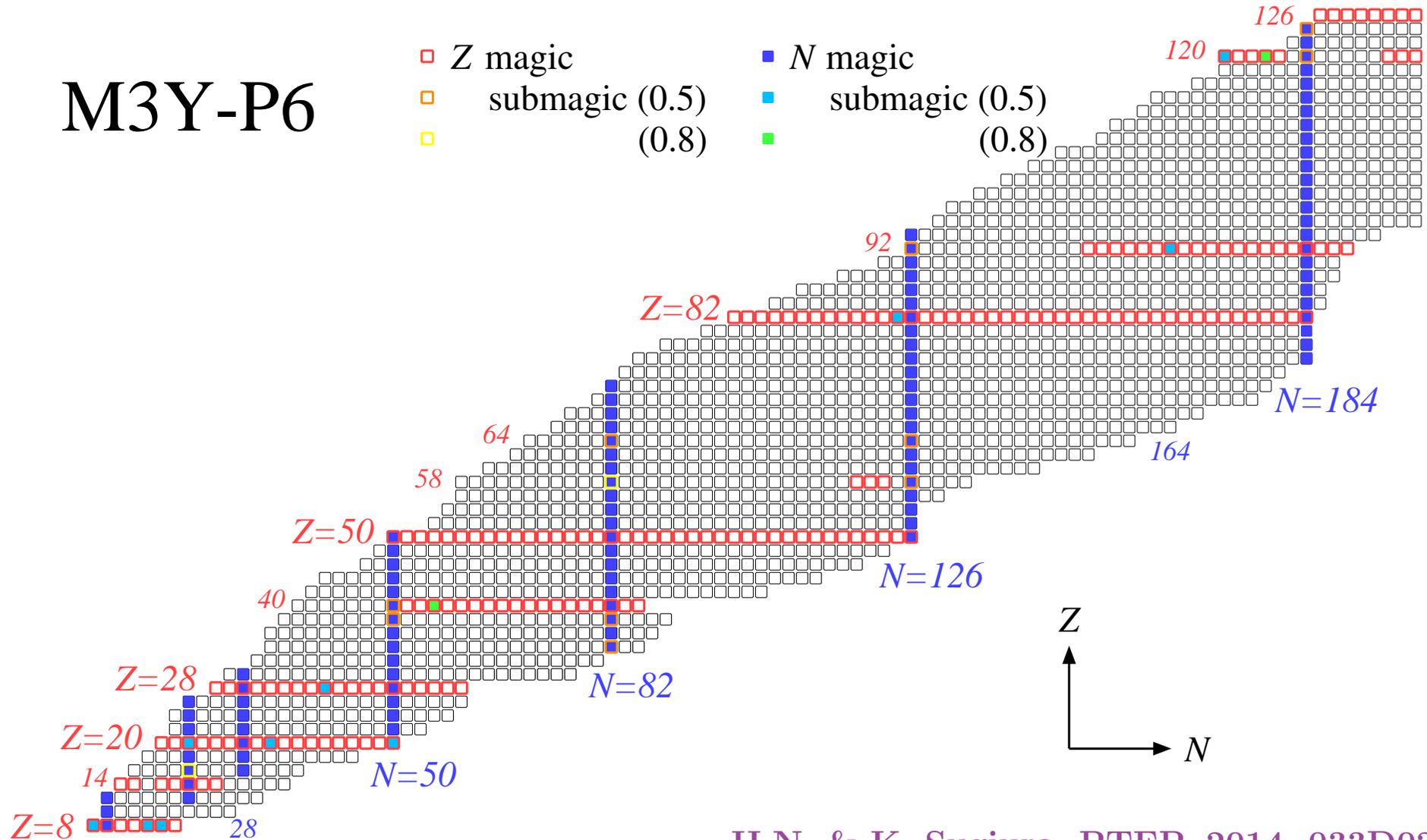
PPNP 120, 103870 ('21)

H.N., PRC 87, 014336 ('13)

★ S.p. pot. @ $\epsilon < 0$ — *e.g.* magic numbers

← quenching of pair correlation

M3Y-P6



H.N. & K. Sugiura, PTEP. 2014, 033D02

⇒ magic # compatible with almost all available data!

(... good s.p. pot. at $\epsilon < 0$)

★ S.p. pot. @ $\epsilon > 0$... $A \rightarrow \infty$ limit (homogeneous nuclear matter)

$$\langle \mathbf{k}\sigma\tau | U | \mathbf{k}\sigma\tau \rangle \approx U_0(\epsilon_N; n) + \tau U_1(\epsilon_N; n) \eta_t; \quad \eta_t := \sum_{\tau'} \tau' n_{\tau'} / n$$

(non-locality $\rightarrow k \rightarrow \epsilon_N$)

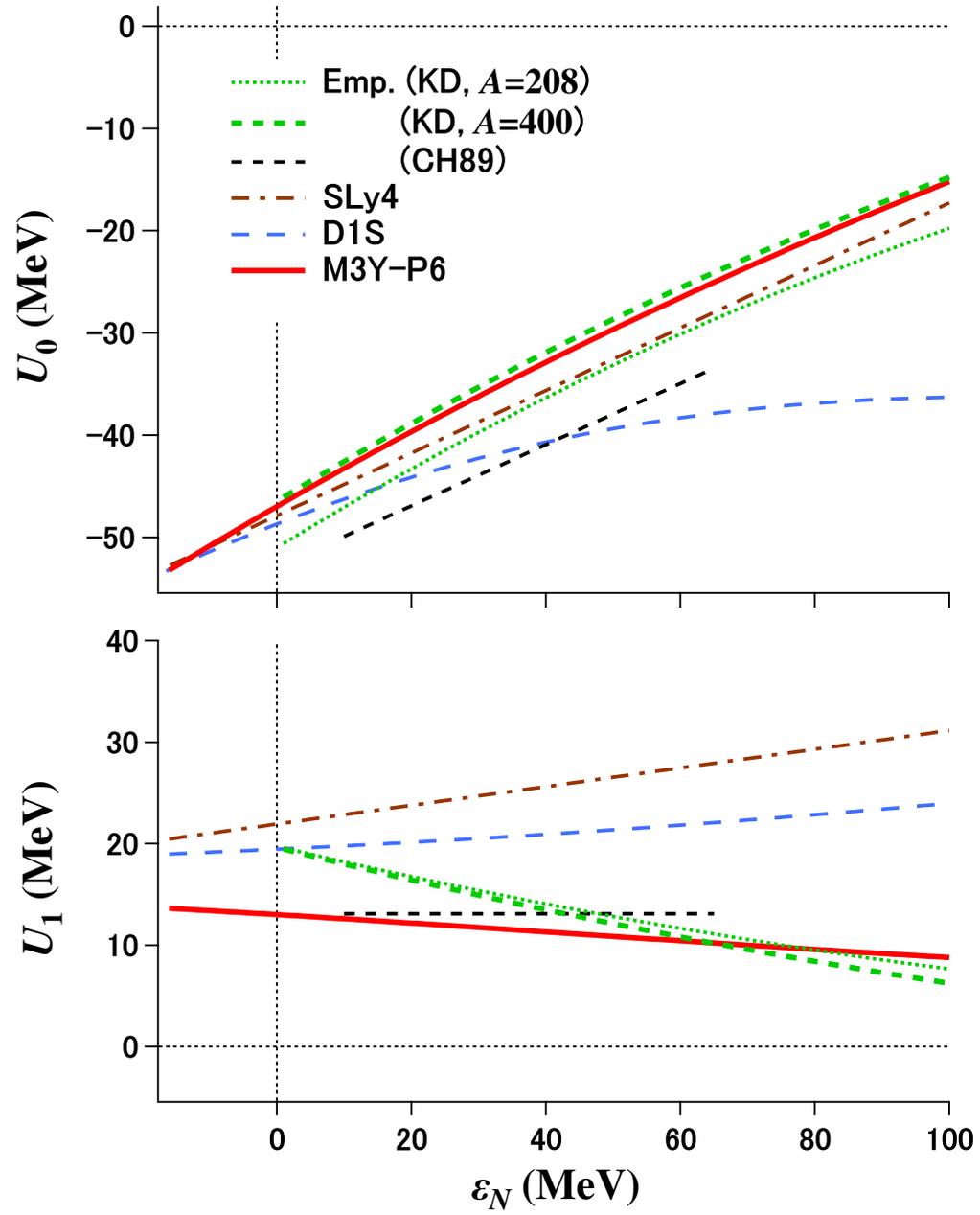
\updownarrow

$$\lim_{A \rightarrow \infty} \mathcal{V}^{\text{emp}}(\mathbf{r} = 0) \approx U_0^{\text{emp}}(\epsilon_N; \rho_0) - \tau U_1^{\text{emp}}(\epsilon_N; \rho_0) \frac{N - Z}{A}; \quad \tau = \begin{cases} +1 & \text{for } p \\ -1 & \text{for } n \end{cases}$$

(local, A - & ϵ_N -dep.)

$$\mathcal{V}^{\text{emp}} \leftarrow \begin{cases} \text{Koning-Delaroche (0.001} \leq \epsilon_N \leq 200 \text{ MeV)} & \text{NPA 713, 231} \\ \text{'CH89' (10} \leq \epsilon_N \leq 65 \text{ MeV)} & \text{Phys. Rep. 201, 57} \end{cases}$$

(KD ... care needed for $A \rightarrow \infty$
 $\therefore (c_1 A)$ term with small $|c_1|$)



★ S.p. pot. @ $\epsilon > 0$... finite (doubly magic) nuclei

$$|\Psi_{A+1}\rangle \approx |\Phi_A\rangle \otimes |\psi_N\rangle$$

$$|\Phi_A\rangle \leftarrow \text{“SCMF” (or KS)} \quad (\epsilon < 0)$$

$$|\psi_N\rangle \leftarrow \mathcal{U} = \mathcal{V}^{\text{SFP}} + i\mathcal{W}^{\text{emp}} \quad (\epsilon > 0)$$

$$\left\{ \begin{array}{l} \mathcal{V}^{\text{SFP}} = U \text{ — self-consistent pot.} \\ \quad \quad \quad \dots \text{ non-local, } \epsilon_N\text{-indep.} \\ \mathcal{W}^{\text{emp}} \leftarrow \text{KD} \dots \text{ local, } A\text{- \& } \epsilon_N\text{-dep. (empirical)} \end{array} \right.$$

$$|\Phi_A\rangle \ \& \ \mathcal{V}^{\text{SFP}}$$

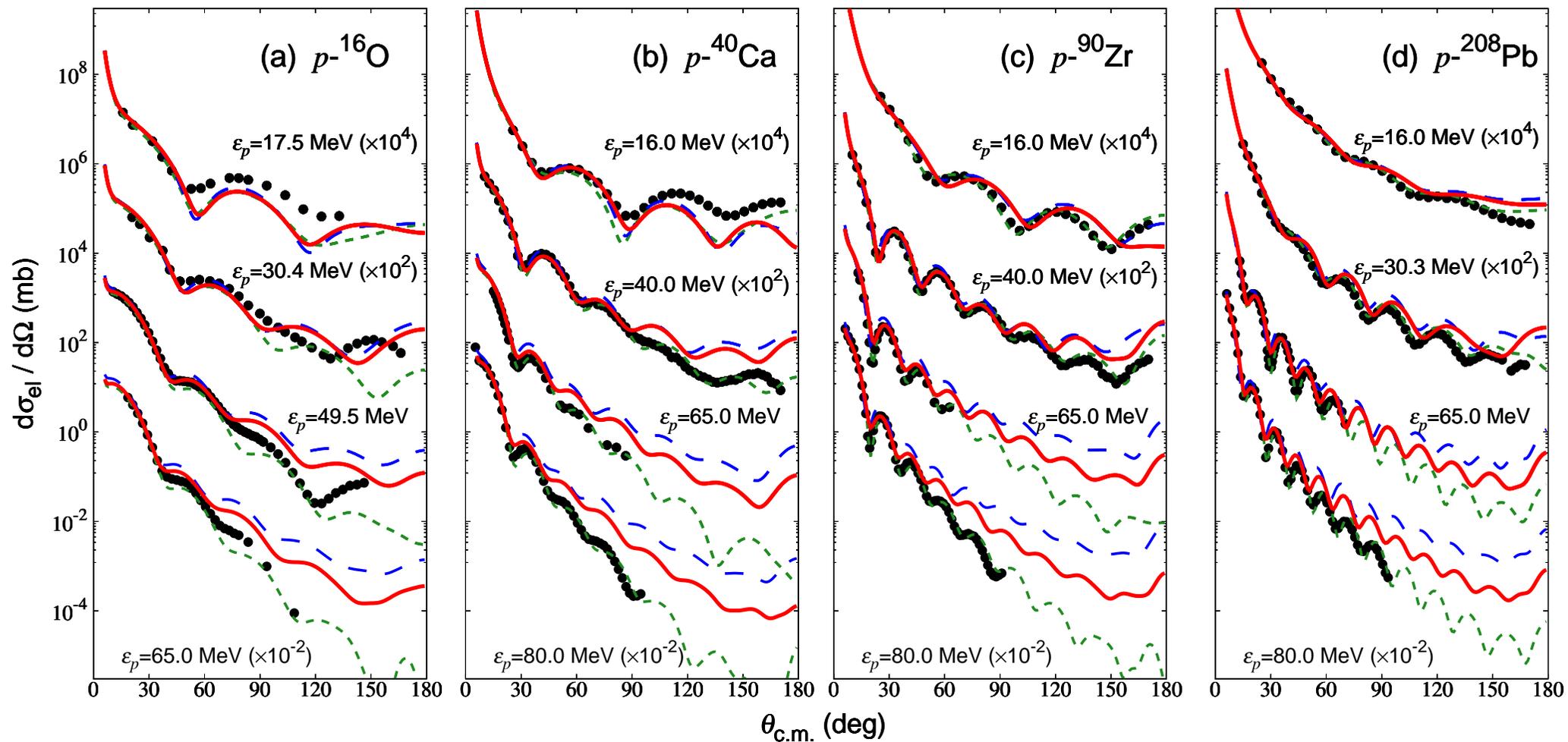


same framework, same eff. int.

\Rightarrow observables $\left(\frac{d\sigma_{\text{el}}}{d\Omega}, \sigma_{\text{reac}} \text{ or } \sigma_{\text{tot}}, A_y, \text{ etc.} \right)$ via **SIDES** code

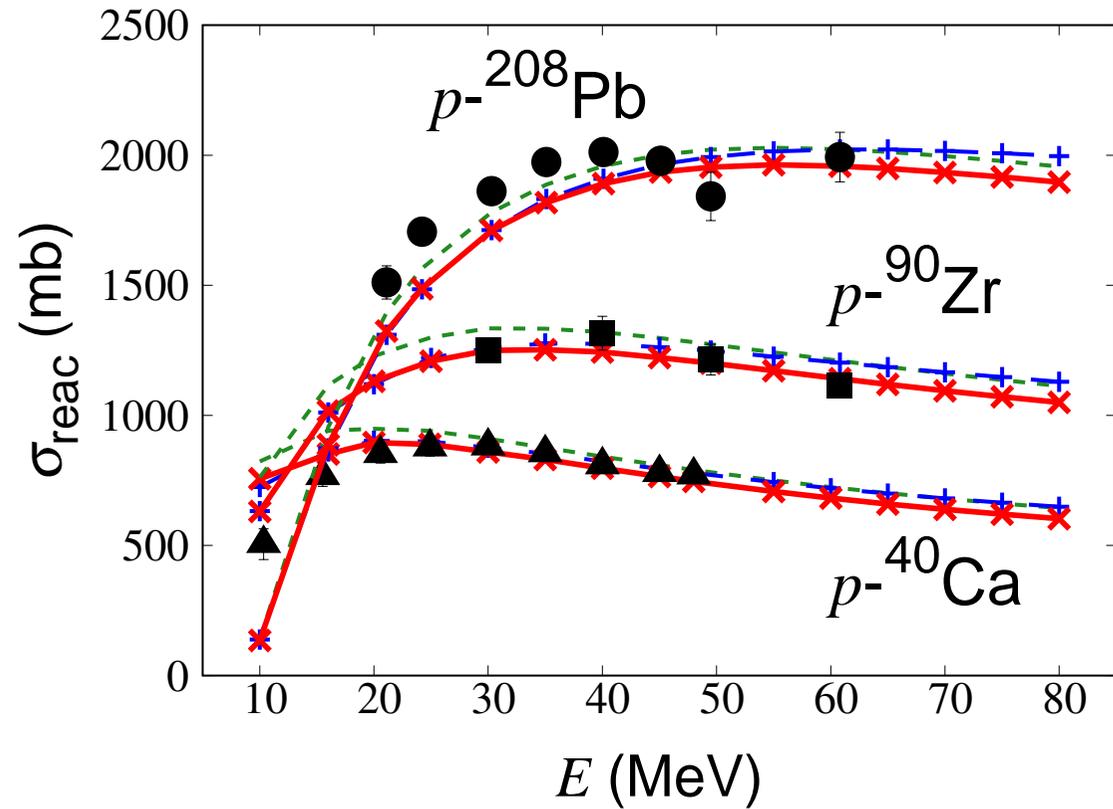
CPC 254, 107340

- cross sections (up to angle-dep.)

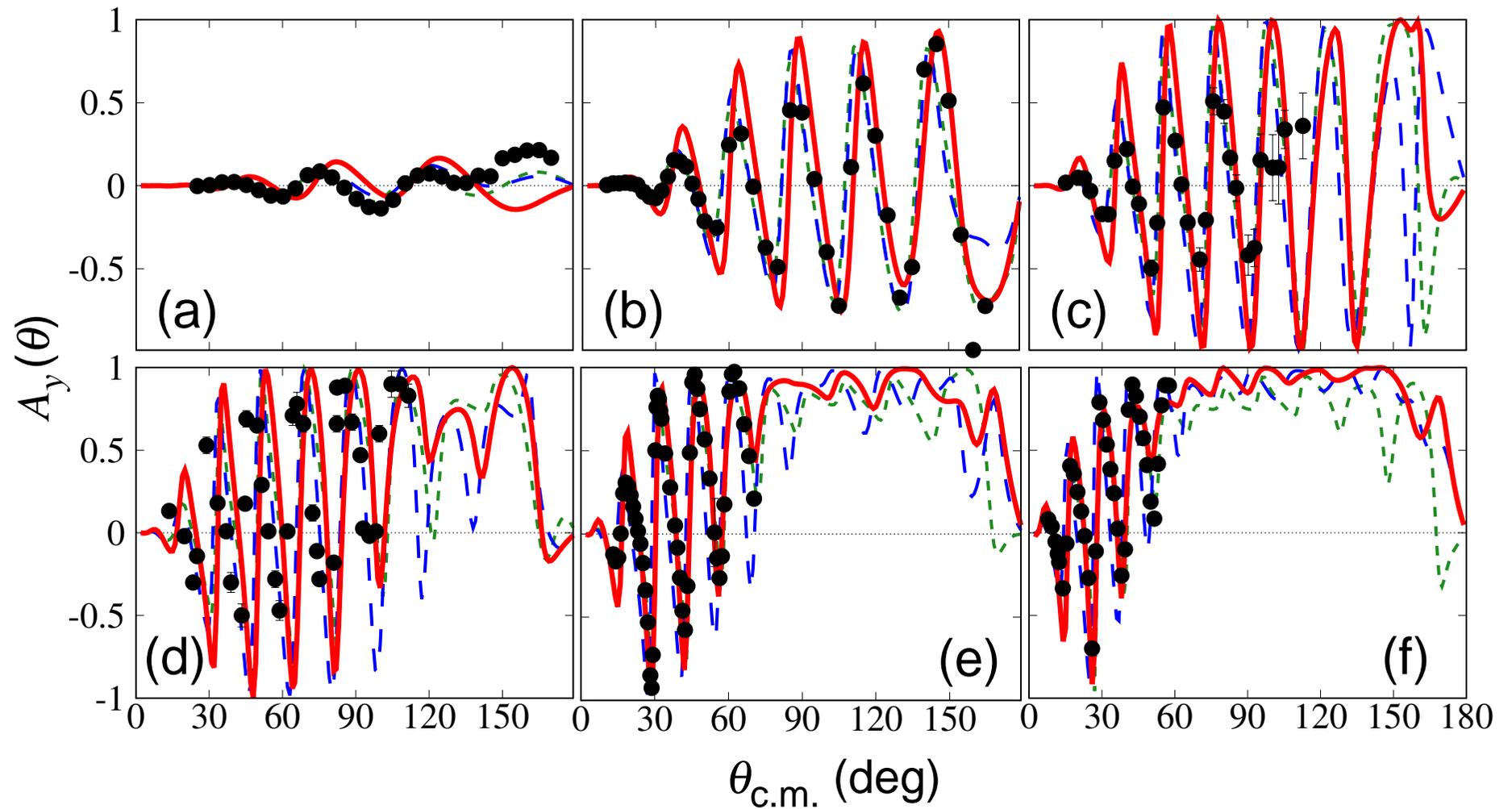


— M3Y-P6 (for ν^{SFP})
 - - - D1S
 - - - KD (ν^{emp})

- validity for \mathcal{W}^{emp} combined with ν^{SFP} ?



- spin-dep. ?

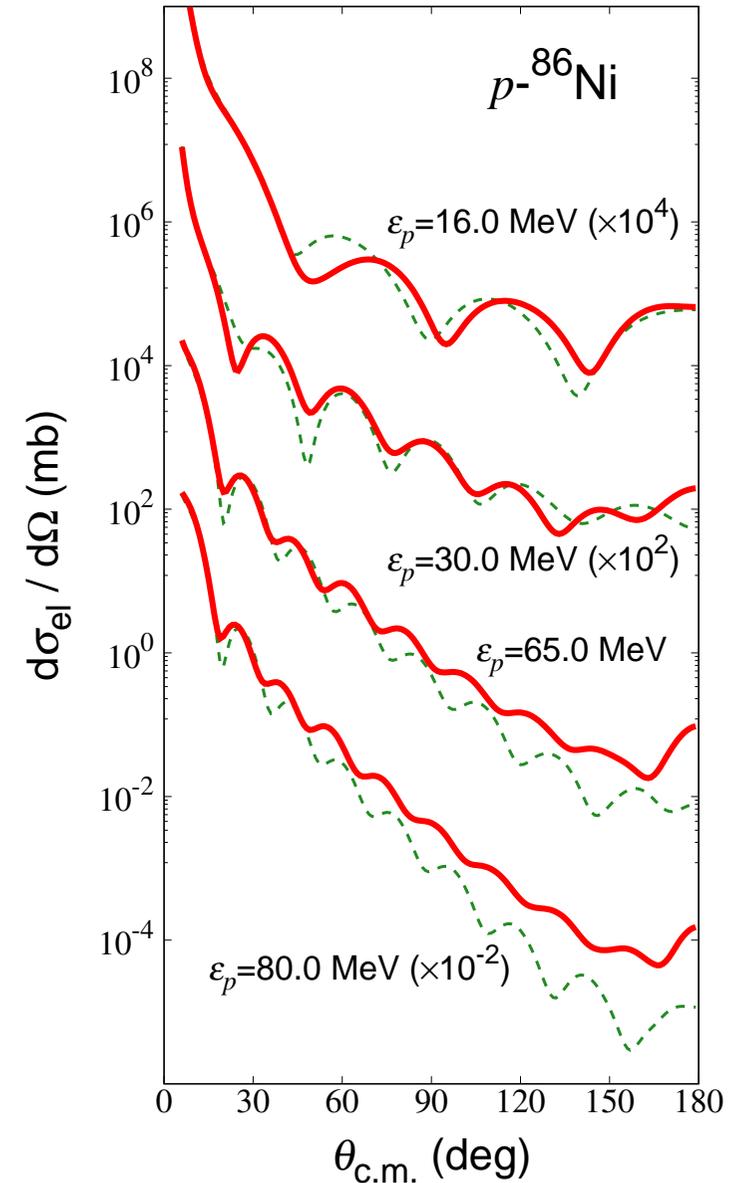
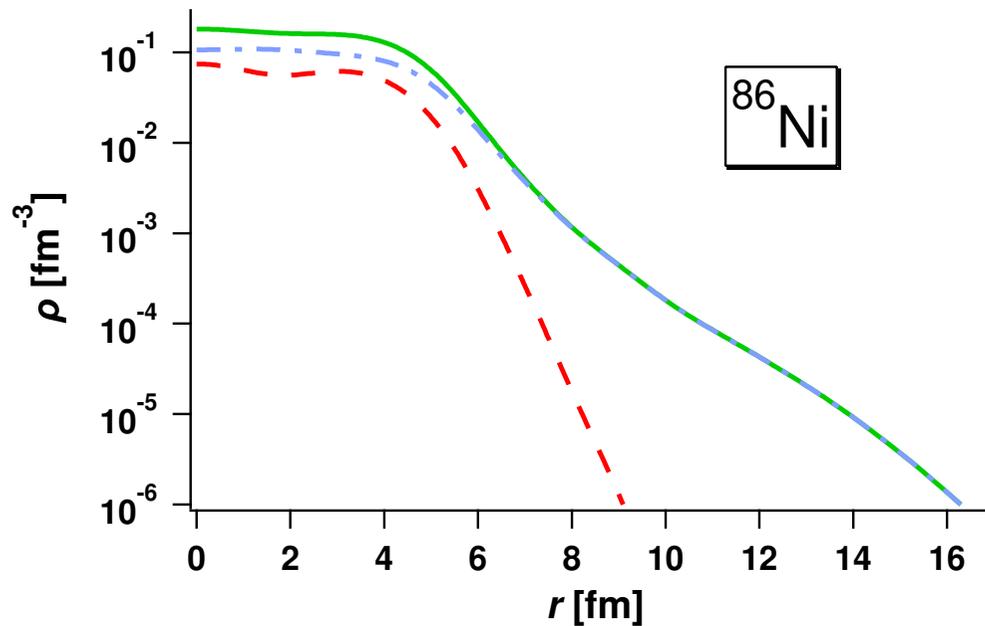


p - ^{208}Pb , $\epsilon_p = 16 - 80$ MeV

\Rightarrow good s.p. pot. in $-20 \lesssim \epsilon \leq (65 - 80)$ MeV !

- elastic scatt. off halo nuclei? ... \mathcal{U}^{emp} — questionable!

→ ^{86}Ni : (nearly) doubly magic with $n2s_{1/2}$ occ. PRC 81, 051302(R)



★ Validity / limitation of (Brieva-Rook) local approx.

NPA 291, 299 & 317; 297, 206

- Brieva-Rook LA ... $\mathcal{V}^{\text{SFP}} \leftarrow n_{p,n}^{(0)}(\mathbf{r})$ **only!**

— valid for “any” A & ϵ_N ?

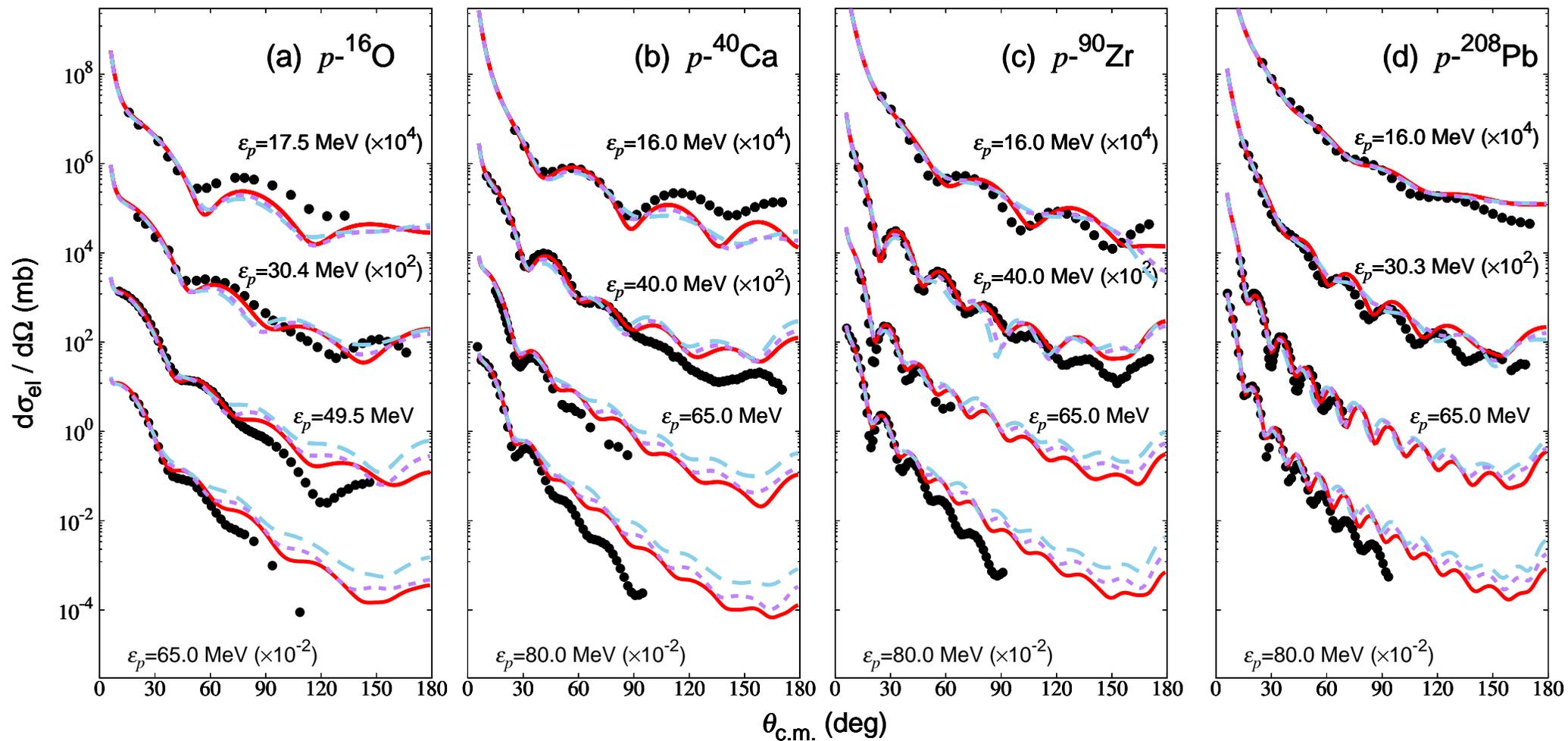
- beyond $n_{p,n}^{(0)}(\mathbf{r})$? $\rightarrow \varrho^{(0)}(\mathbf{r}, \mathbf{r}')$ (1-b. DM)

advantage of PW ... $\left\{ \begin{array}{l} \varrho^{(0)} \text{ within int. range: well examined!} \\ \text{influence of } \hat{v}_{ij}^{(\text{LS})} \text{ (\& } \hat{v}_{ij}^{(\text{TN})}) \\ \text{can be investigated} \end{array} \right.$

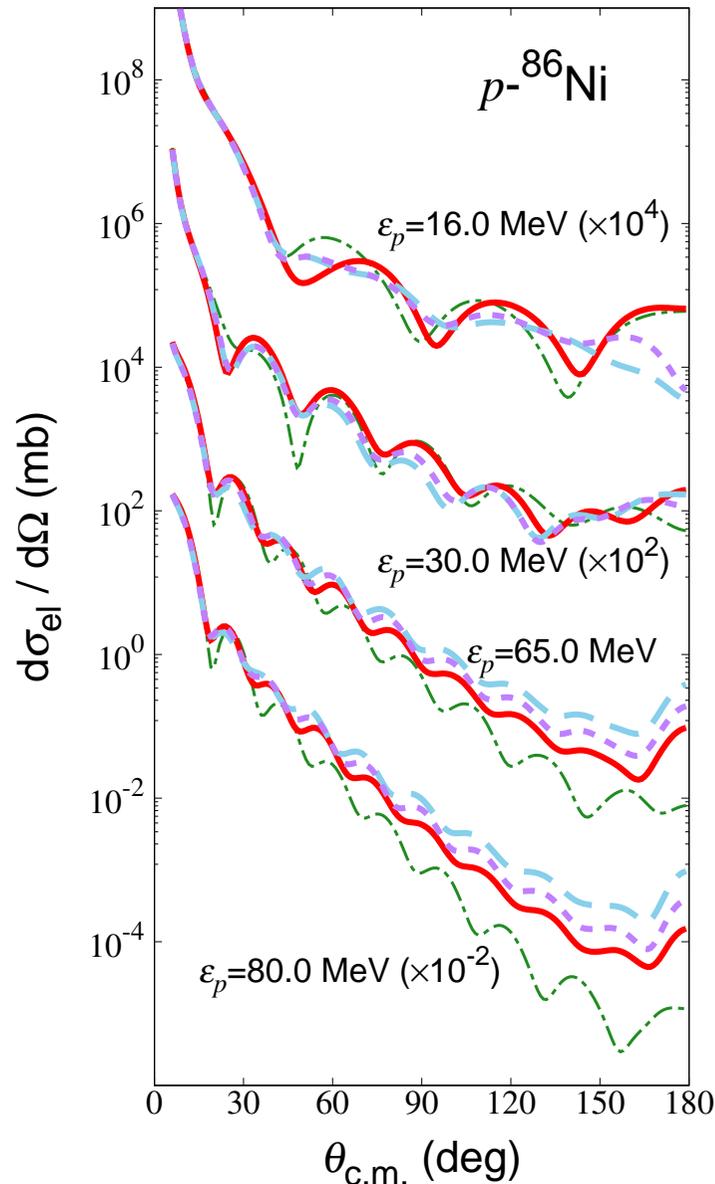
cf. H.F. Arellano *et al.*, PRC 42, 652

K. Minomo *et al.*, JPG 37, 085011

• cross sections (up to angle-dep.)



- scatt. off halo nuclei?



- exact (non-local SFP)
- - - LA for $\hat{v}^{(C)}$
- - - LA for $\hat{v}^{(C)} + \hat{v}^{(LS)}$
- · - KD (empirical)

- o notable influence of LA

@ $\varepsilon_p = 16 \text{ MeV}$

↔ halo

- o coupling to continuum

— \mathcal{V}^{SFP} good enough?

→ future exp.?

V. Summary & perspective

★ Self-consistent single-nucleon pot.

... extension of KS approach w.r.t. ϵ

→ target w.f. & \mathcal{V}^{SFP} (non-local, ϵ_N -indep.)

↓
 N - A scatt. ($A \rightarrow \infty$ limit & finite nuclei)

- Wide energy range ($\epsilon \lesssim 80$ MeV) can be covered by a single energy-indep. int.! (— demonstrated by M3Y-P6)
 - ... power of KS approach w/ semi-realistic int.
 - ↪ filling the gap b/w micro. & phenom. int. (“fine tuning”)
- Optical pot. @ unstable nuclei
 - ... beyond empirical pot. *e.g.* halo effects
- (Brieva-Rook) LA
 - insufficient @ large q ($\epsilon_N \lesssim 80$ MeV)
 - significant influence of LA for $\hat{v}^{(\text{LS})}$
 - insufficient for halo nuclei (even at low q)

★ Implication

- **Extendability with enhanced analyticity of $E^{\text{KS}}[\rho]$**
 (\leftrightarrow v -representability)
 \hookrightarrow **collection of well-examined s.p. pot. & levels up to high- ϵ**
- **Future extension to finite- T ?** (optimistic view)
existence of $F_T^{\text{KS}}[\rho] = (E - TS)^{\text{KS}}[\rho]$ @ each T
 $\leftarrow \min_{\{\Psi\} \rightarrow Q} F_T : \text{constrained search}$
dominance of s.p. d.o.f. @ higher- $T \rightarrow$ rationality of $F_T^{\text{KS}}[\rho]$
— analyticity w.r.t. T ? ... U^{KS} @ high- ϵ ?
 \hookrightarrow **EoS @ finite- T consistent with exp. data**
cf. detailed balance \rightarrow no absorption @ equilibrium
 $\epsilon \lesssim 80 \text{ MeV} \rightarrow T \lesssim 30 \text{ MeV} \Rightarrow$ **applicability to supernovae !(?)**