Extension of Kohn-Sham approach to low- to intermediate-energy nucleon-nucleus elastic scattering

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H.N. & K. Ishida, PRC 109, 044614; 110, 019901(E)
K. Ishida & H.N., tbp in PRC (arXiv:2504.05664)

I. Introduction

★ **"Minimal composition" (≈ "essence") of Kohn-Sham theory**

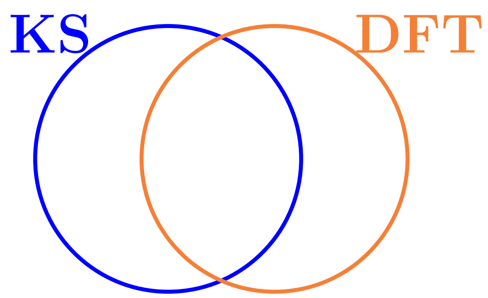
H.N., Phys. Scr. 98, 105007; talk @ DFT2024

$$E[\varrho^{\mathrm{KS}}] \quad \leftarrow \quad E\big[\boldsymbol{Q}[\varrho]\big] = \min_{\Psi \to \boldsymbol{Q}} E[\Psi]$$

$\boldsymbol{Q}$: **principal variables**

$\big(n(\boldsymbol{r}) \in \boldsymbol{Q}$ ··· **unnecessary !**$\big)$

ϱ : **1-b. DM**



★ **"v-representability" = differentiability** $\leftrightarrow$ **universality of** $E[\varrho^{\mathrm{KS}}]$

— **should not be disregarded !**

★ **KS orbitals ··· artifact ?** $\rightarrow$ **"quasiparticle" à la Landau**

(= dressed particle)

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

$$\big(H \;\rightarrow\; h^{\mathrm{KS}} + (H - h^{\mathrm{KS}})\,e^{\eta t}\big)$$

$\because$) **adiabatic theorem**

$$= \mathcal{U}(0,-\infty)\Big[\prod_{i=1}^{N} a_i^{\mathrm{KS}\,\dagger}|0\rangle\Big] = \prod_{i=1}^{N} \underbrace{\big[\mathcal{U}(0,-\infty)\,a_i^{\mathrm{KS}\,\dagger}\,\mathcal{U}^{-1}(0,-\infty)\big]}_{\text{"quasiparticle"}}|0\rangle$$

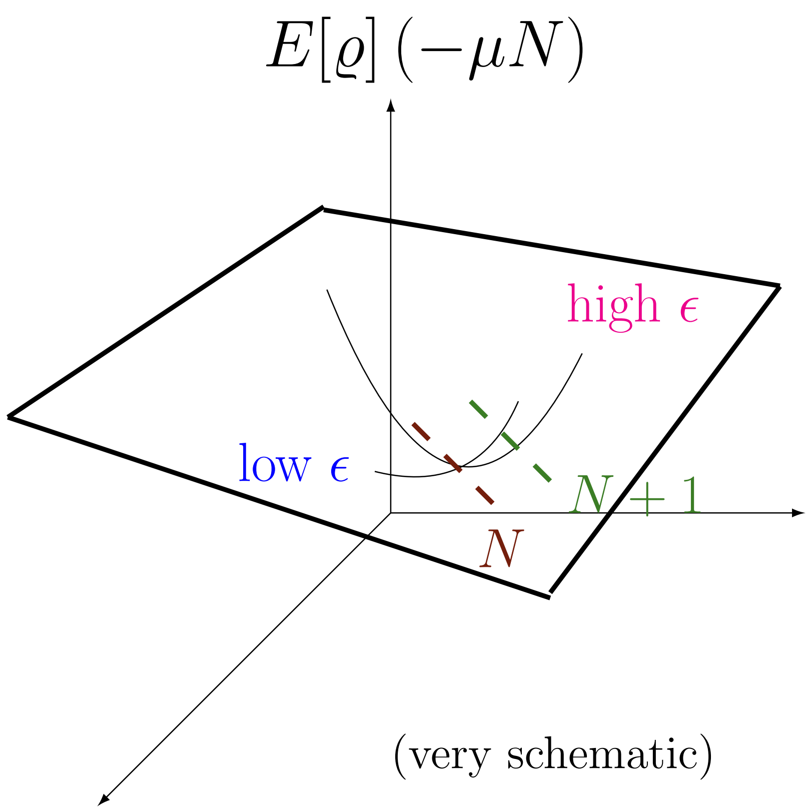
★ Extension of KS approach to s.p. states at $\epsilon > 0$

structure of $E[\varrho^{\mathrm{KS}}]$? (— **complicated manifold**)

$$h^{\mathrm{KS}} = \frac{\delta E}{\delta \varrho^{\mathrm{KS}}} = \frac{\boldsymbol{p}^2}{2M} + U^{\mathrm{KS}} \rightarrow \text{s.p. states}$$

$\uparrow$ **containing many-body corr.**

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



U^{KS} **at** $\epsilon > 0$ $\leftrightarrow$ **real part of optical pot.** $\mathcal{V}^{\mathrm{SFP}}$

many-body corr. $\leftrightarrow$ **"dynamical pol. effect"**

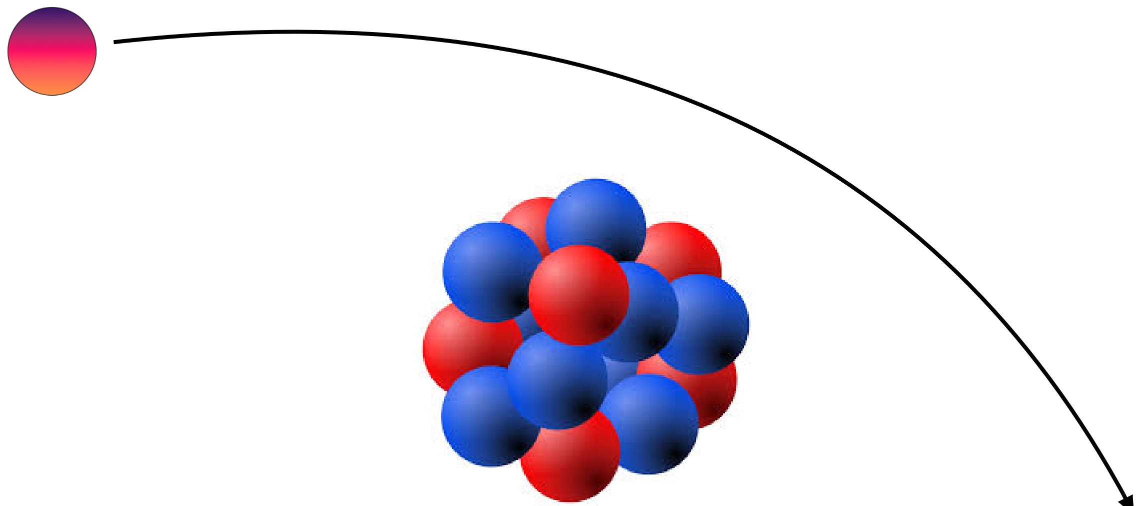
imag. part ? — beyond MF (KS)

cf. $\delta^2 E/\delta\varrho^2$ $\leftrightarrow$ **RPA or TDKS**

★ N-A scattering

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

channel branching — beyond KS



“KS approach” to elastic channel : $E[\varrho^{\rm KS}] \quad \to \quad \left\{ \begin{array}{l} |\Psi_A\rangle \approx |\Phi_A^{\rm KS}\rangle \\ (\mathcal{V}^{\rm SFP} \to)\ |\psi_N\rangle \end{array} \right.$

(dressed nucleon)

II. Self-consistent single-nucleon potential

★ Self-consistent pot. from eff. int. (or EDF)

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

$$\rightarrow \quad h|\alpha^{(0)}\rangle = \epsilon_{\alpha(0)}|\alpha^{(0)}\rangle \quad \textbf{with} \quad h = \sum_{\alpha\alpha'} |\alpha\rangle \left.\frac{\delta E}{\delta\varrho_{\alpha'\alpha}}\right|_{\varrho^{(0)}} \langle\alpha'| = \frac{\boldsymbol{p}^2}{2M} + U$$

input : eff. int. (or EDF) $\cdots \quad \hat{v}_{\rm eff} = \sum_i C_i[n(\boldsymbol{r})]\cdot\hat{w}_i$

$\hat{w}_i$ **: two-body operator**

$$\rightarrow \quad U|\alpha\rangle = \sum_i \sum_{\beta\beta'} \big\langle *\beta\big|C_i[n^{(0)}(\boldsymbol{R}_{\alpha\beta})]\cdot\hat{w}_i\big|\alpha\beta'\big\rangle\, \varrho^{(0)}_{\beta\beta'}$$

$$+\frac{1}{2}|\alpha\rangle \sum_i \sum_{\alpha''\alpha'\beta\beta'} C_i'[n^{(0)}(\boldsymbol{r}_\alpha)]\, \big\langle\alpha''\beta\big|\delta(\boldsymbol{r}_\alpha - \boldsymbol{R}_{\alpha''\beta})\cdot\hat{w}_i\big|\alpha'\beta'\big\rangle\, \varrho^{(0)}_{\alpha'\alpha''}\, \varrho^{(0)}_{\beta'\beta}$$

$$|\Phi_A^{\rm KS}\rangle \;\leftrightarrow\; \varrho^{(0)}$$

★ **Finite-range eff. int. (↔ non-local EDF)**

— possibly important to cover high ϵ

→ { **new code applicable to non-local optical pot. → available**
complete formulae for U^{KS} → derived }

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

M3Y int. ⋯ **Yukawa function → fit to G-matrix (@ $n \approx n_0/3$)**

'**M3Y-Pn**' **H.N., P.R.C 68, 014316 ('03)**

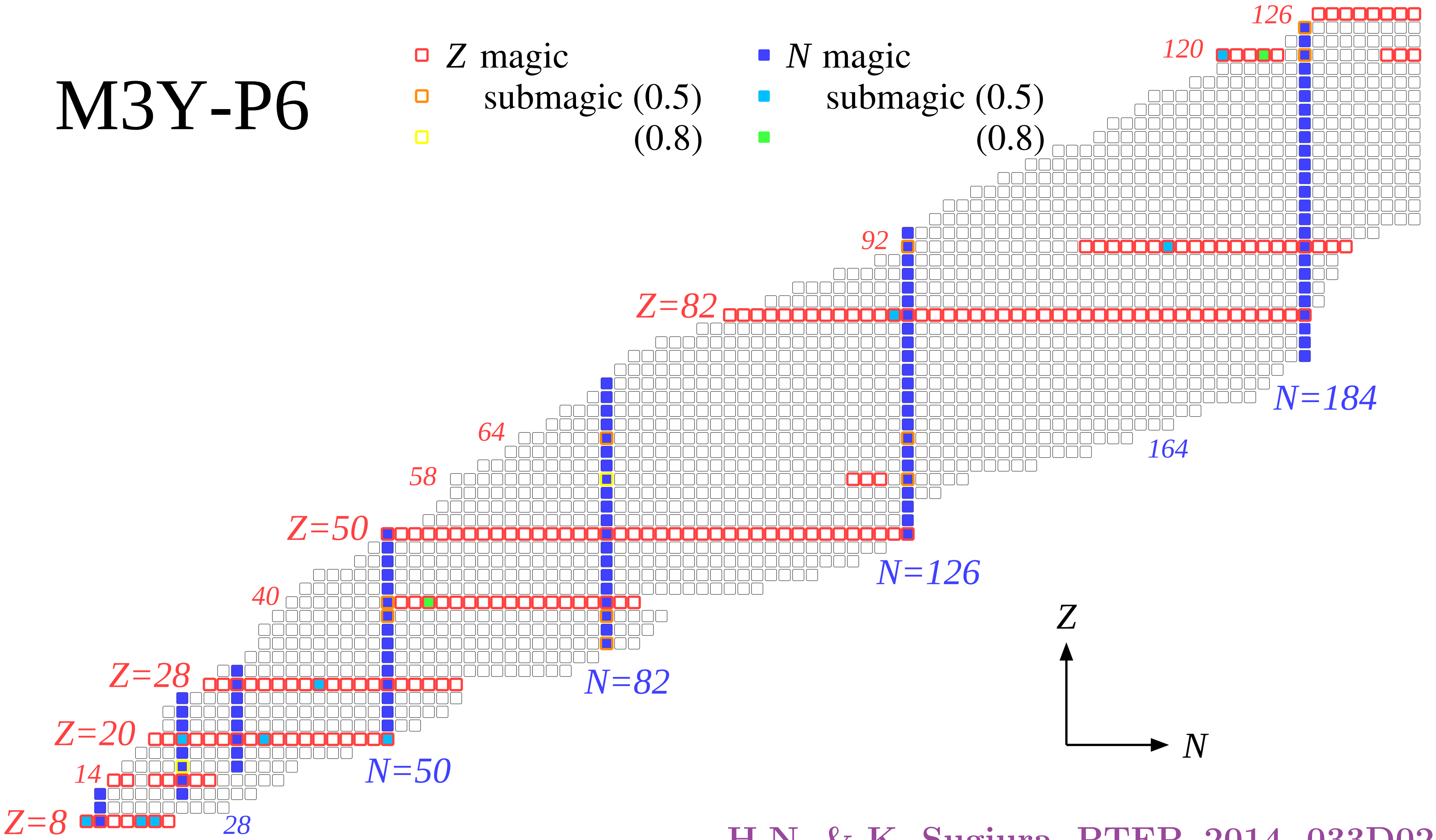
- **modifying M3Y-Paris** { **replace short-range part of $\hat{v}^{(\mathrm{C})}$ by $\hat{v}^{(\mathrm{C}\rho)}$**
enhance $\hat{v}^{(\mathrm{LS})}$ (↔ ℓs splitting) }
- **keeping $\hat{v}_{\mathrm{OPEP}}^{(\mathrm{C})}$ (longest-range part)**
- **no change for $\hat{v}^{(\mathrm{TN})}$ from M3Y-Paris — realistic tensor force**

M3Y-P6 : H.N., P.R.C 87, 014336 ('13); I.J.M.P.E 29, 1930008 ('20)

(Gogny-D1S & Skyrme-SLy4 ⋯ **for comparison)**

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

← quenching of pair correlation



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

⇒ magic # compatible with almost all available data !

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

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

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

(non-locality $\to k \to \epsilon_N$**)**

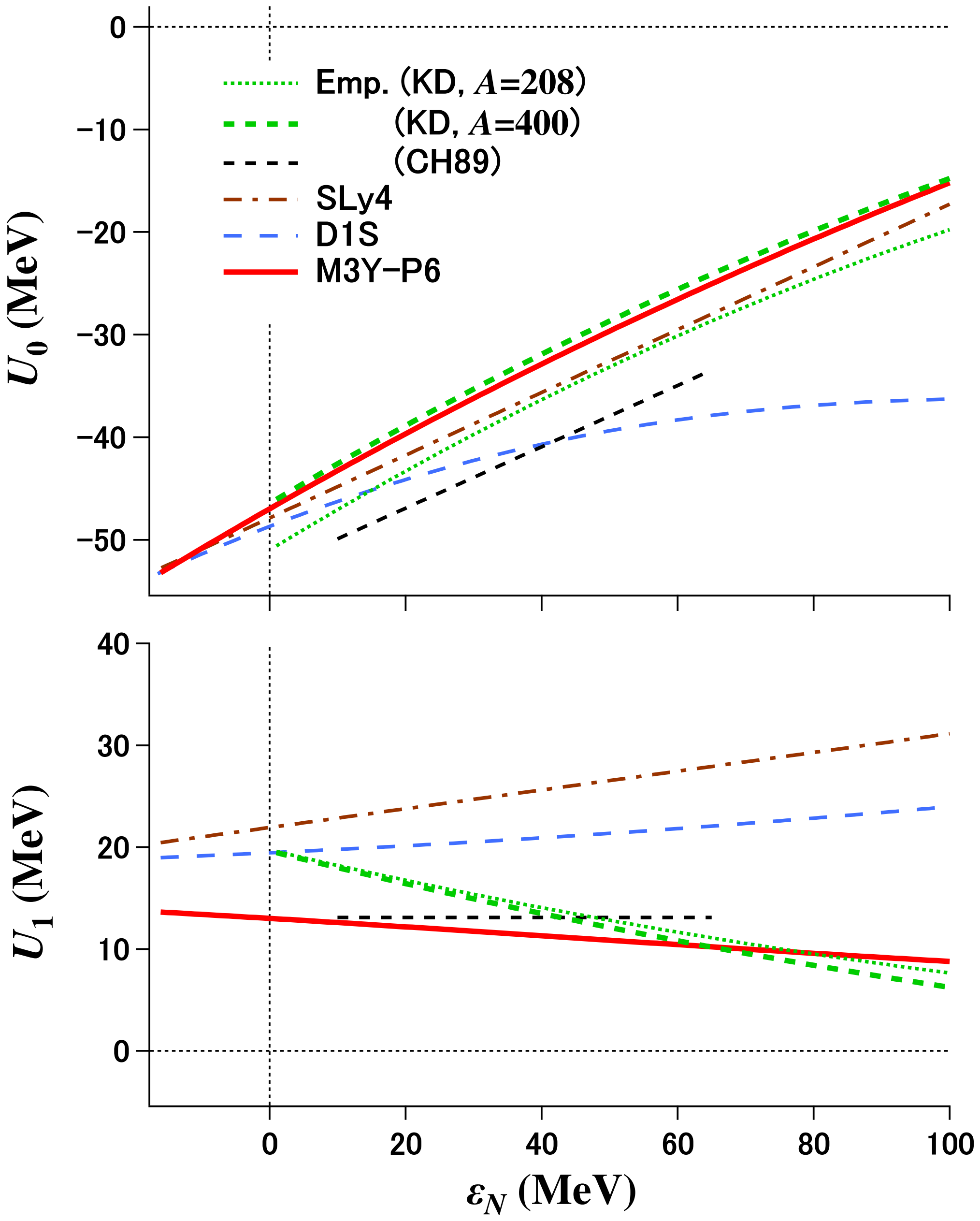
$$\updownarrow$$

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

(local, A**- &** ϵ_N**-dep.)**

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

$$\left(\begin{array}{l} \textbf{KD} \cdots \textbf{ care needed for } A \to \infty \\ \quad \because\ (c_1 A) \textbf{ term with small } |c_1| \end{array} \right)$$



Emp. (KD, A=208)
(KD, A=400)
(CH89)
SLy4
D1S
M3Y-P6
U0 (MeV)
U1 (MeV)
εN (MeV)
0
−10
−20
−30
−40
−50
40
30
20
10
0
0
20
40
60
80
100

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

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

$|\Phi_A\rangle \leftarrow$ **"SCMF" (or KS)** $(\epsilon < 0)$

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

$\mathcal{V}^{\mathrm{SFP}} = U$ — **self-consistent pot.**

$\cdots$ **non-local, ϵ_N-indep.**

$\mathcal{W}^{\mathrm{emp}} \leftarrow$ **KD** $\cdots$ **local, A- & ϵ_N-dep. (empirical)**

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

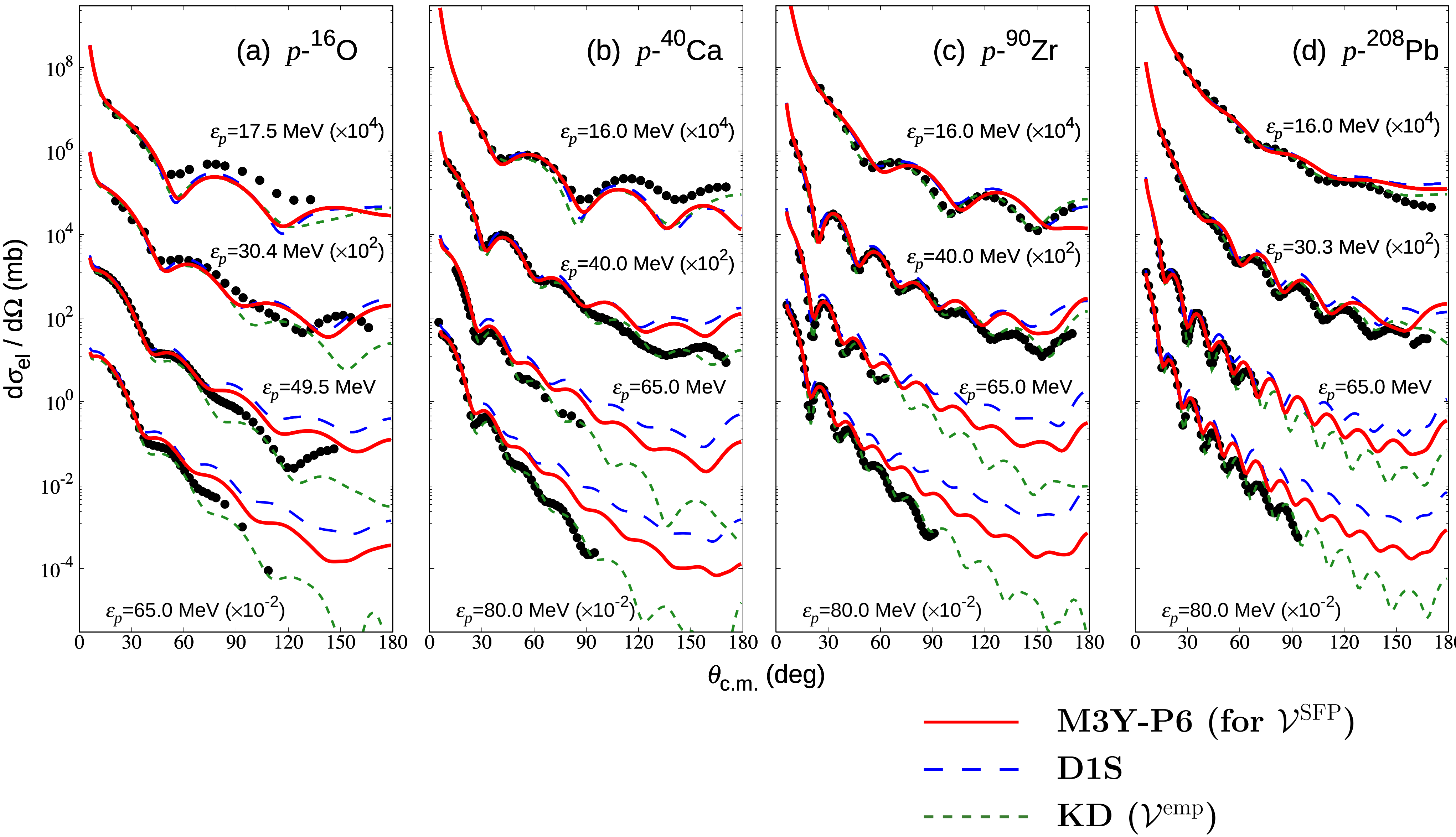
↖

same framework, same eff. int.

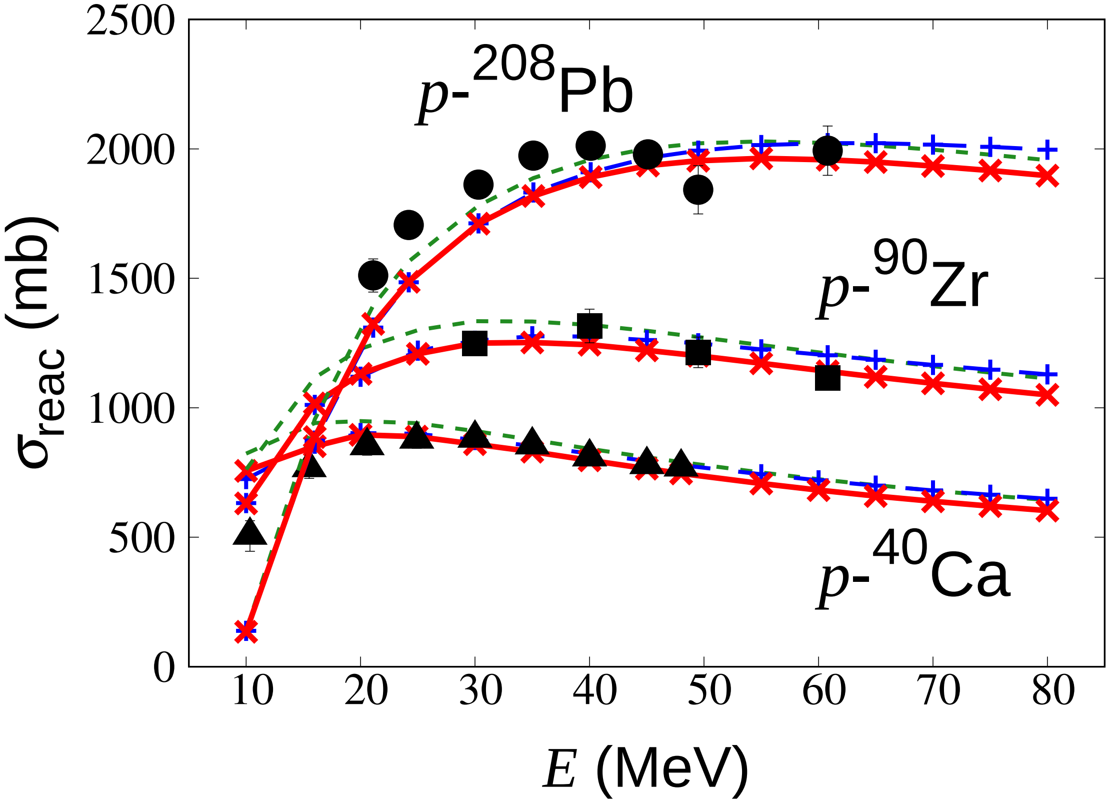
$\Rightarrow$ **observables** $\left(\frac{d\sigma_{\mathrm{el}}}{d\Omega}, \sigma_{\mathrm{reac}}\ \textbf{or}\ \sigma_{\mathrm{tot}}, A_y, \textbf{\textit{etc.}}\right)$ **via SIDES code**

CPC 254, 107340

- **cross sections (up to angle-dep.)**

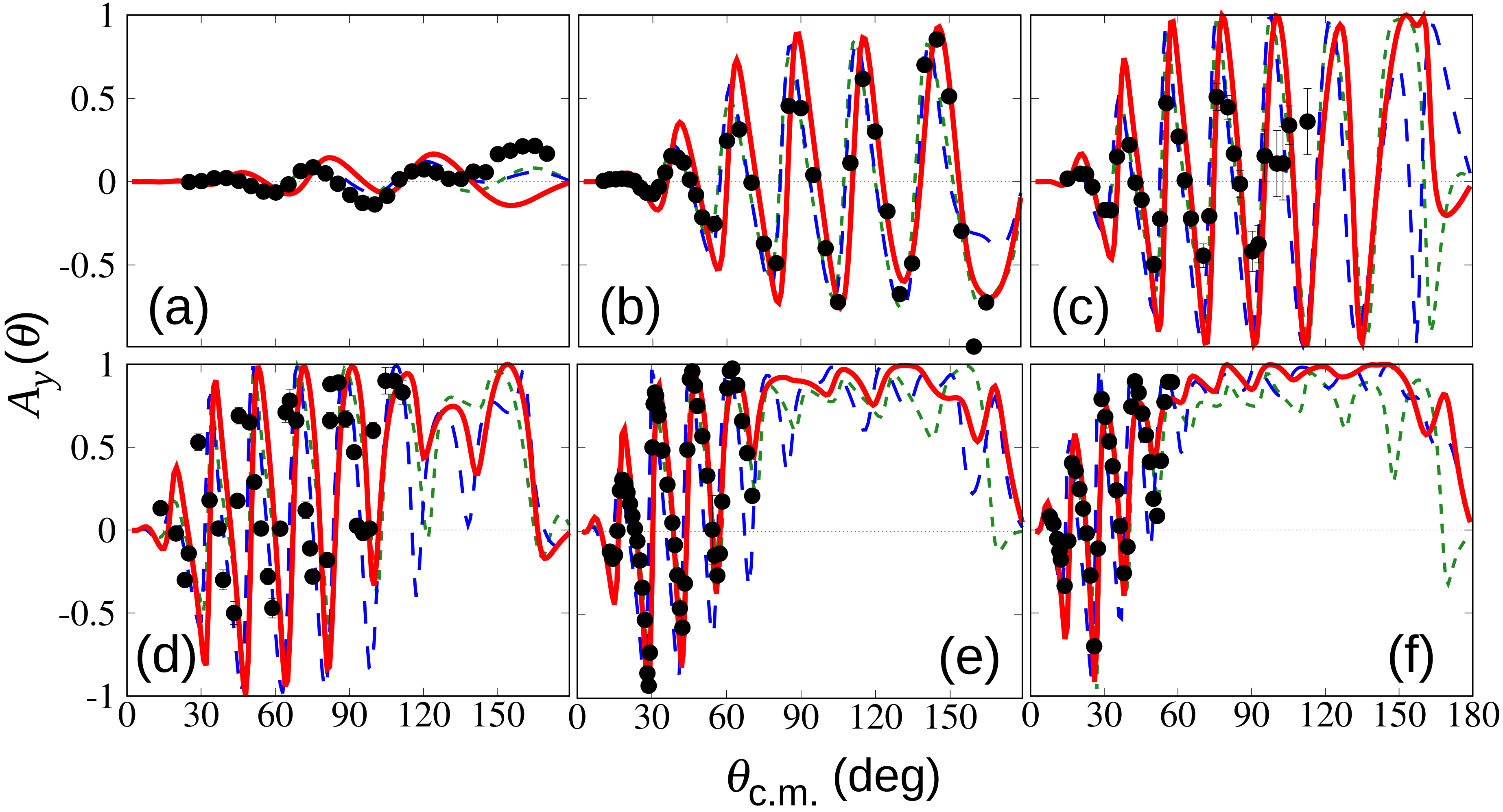


- **validity for** $\mathcal{W}^{\rm emp}$ **combined with** $\mathcal{V}^{\rm SFP}$ **?**



$\Longrightarrow$ **good s.p. pot. in** $-20 \lesssim \epsilon \leq (65-80)\,\mathrm{MeV}$ **!** $(\rightarrow T \lesssim 30\,\mathrm{MeV})$

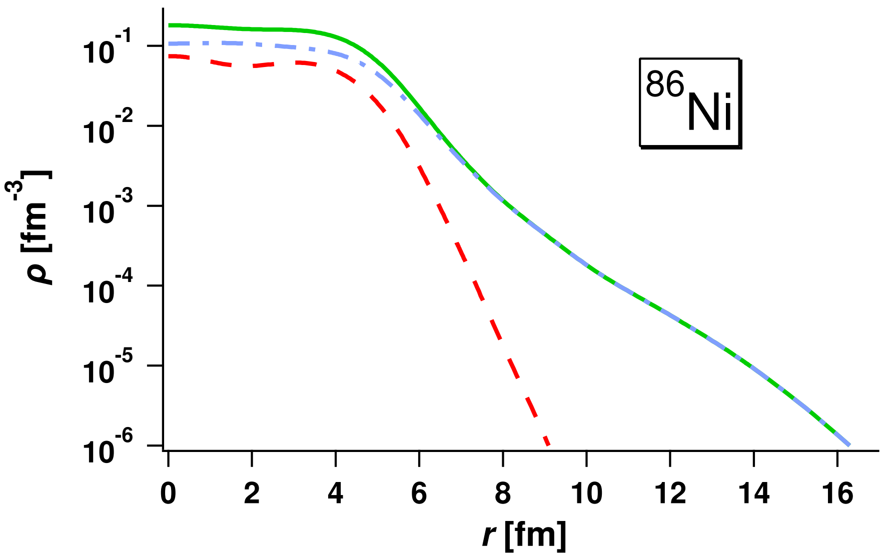
- **spin-dep. ?**

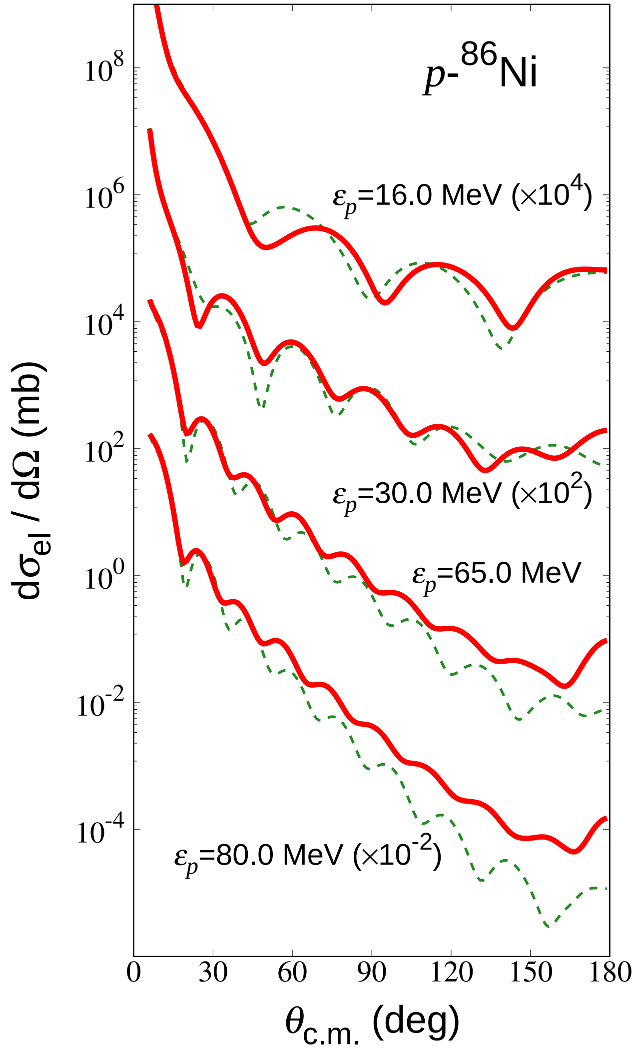


p-^{208}**Pb,** $\epsilon_p = 16 - 80\,\text{MeV}$

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

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





V. Summary & perspective

★ **Self-consistent single-nucleon pot.** $\cdots$ **extended w.r.t.** ϵ

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

$\searrow$

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

- **Wide energy range (**$\epsilon \lesssim 80\,\mathrm{MeV}$**) can be covered by a single energy-indep. int.!** **(— demonstrated by M3Y-P6)**
- **Optical pot. @ unstable nuclei**
  $\cdots$ **(possibly) beyond empirical pot.** ***e.g.*** **halo effects**

★ **Implication**

- **Extendability with enhanced analyticity of** $E[\varrho^{\mathrm{KS}}]$
  ($\leftrightarrow$ v**-representability)**

$\hookrightarrow$ **collection of well-examined s.p. pot. & levels up to high-**ϵ

- **Future extension to finite-T ?** **(optimistic view)**

  existence of $F_T[\varrho^{\rm KS}] = (E - TS)[\varrho^{\rm KS}]$ **@ each** T

  $\leftarrow \min_{\{\Psi\}\to \boldsymbol{Q}} F_T$ **: constrained search**

  dominance of s.p. d.o.f. @ higher-T $\rightarrow$ **rationality of** $F_T[\varrho^{\rm KS}]$

  — analyticity w.r.t. T **?** $\cdots$ $U^{\rm KS}$ **@ high-**ϵ **?**

$\hookrightarrow$ **EoS @ finite-**T **consistent with exp. data**

cf. detailed balance $\rightarrow$ **no absorption @ equilibrium**

$\epsilon \lesssim 80\,\mathrm{MeV} \rightarrow T \lesssim 30\,\mathrm{MeV}$ $\Rightarrow$ **applicability to supernovae !(?)**