# Oddziaływania efektywne niezależne od gęstości

#### Jacek Dobaczewski University of Warsaw & University of Jyväskylä





#### with Karim Bennaceur and Francesco Raimondi

Seminarium "Struktura jądra atomowego" Uniwersytet Warszawski 16 maja 2013





YVÄSKYLÄN YLIOPISTO



# Outline

- **1. Introduction effective theories in physics**
- 2. Energy density functionals in nuclear physics
- 3. Effective interactions vs. functional

generators

- 4. Regularized pseudopotentials
- 5. Three-body forces vs. density-dependent terms
- 6. New functionals without density dependence
- 7. Conclusions





JYVÄSKYLÄN YLIOPISTO





YVÄSKYLÄN YLIOPISTO

An effective theory (ET) is a theory which "effectively" captures what is physically relevant in a given domain. The most appropriate description of particle interactions in the language of quantum field theory (QFT) depends on the energy at which the interactions are studied. **Objective reductionism** (Weinberg): the convergence of arrows of scientific explanation. **Emergence (Anderson): at each** new level of complexity entirely new properties appear and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other.

Elena Castellani, physics/0101039



### Hydrogen atom perturbed near the center



**Relative errors in the S**wave binding energies are plotted versus: (i) the binding energy for the Coulomb theory (ii) the Coulomb theory augmented with a delta function in first-order perturbation theory (iii) the non-perturbative effective theory through a<sup>2</sup>, and (iv) the effective theory through a<sup>4</sup>.







# Phase shifts in the low-momentum expansion











VÄSKYLÄN V



## **Phenomenological functional generators**

• Gogny\*

$$V(ec{r}_1ec{r}_2;ec{r}_1'ec{r}_2') = \delta(ec{r}_1 - ec{r}_1')\delta(ec{r}_2 - ec{r}_2')V(ec{r}_1 - ec{r}_2),$$

where,

$$V(ec{r_1}-ec{r_2}) = \sum_{i=1,2} e^{-(ec{r_1}-ec{r_2})^2/\mu_i^2} imes (W_i + B_i P_\sigma - H_i P_ au - M_i P_\sigma P_ au) 
onumber \ + t_3(1+P_\sigma)\delta(ec{r_1}-ec{r_2})
ho^{1/3} \left[rac{1}{2}(ec{r_1}+ec{r_2})
ight].$$

 $P_{\sigma} = \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$  and  $P_{\tau} = \frac{1}{2}(1 + \vec{\tau}_1 \cdot \vec{\tau}_2)$  are, respectively, the spin and isospin exchange operators of particles 1 and 2,  $\rho(\vec{r})$  is the total density of the system at point  $\vec{r}$ , and  $\mu_i = 0.7$  and  $1.2 \,\mathrm{fm}$ ,  $W_i$ ,  $B_i$ ,  $H_i$ ,  $M_i$ , and  $t_3$  are parameters.

#### • Skyrme\*

$$\begin{split} V(\vec{r}_{1}\vec{r}_{2};\vec{r}_{1}'\vec{r}_{2}') &= \left\{ t_{0}(1+x_{0}P^{\sigma}) + \frac{1}{6}t_{3}(1+x_{3}P^{\sigma})\rho^{\alpha}\left(\frac{1}{2}(\vec{r}_{1}+\vec{r}_{2})\right) \right. \\ &+ \frac{1}{2}t_{1}(1+x_{1}P^{\sigma})[\vec{k'}^{*2} + \vec{k}^{2}] + t_{2}(1+x_{2}P^{\sigma})\vec{k'}^{*}\cdot\vec{k} \right\} \delta(\vec{r}_{1} - \vec{r}_{1}')\delta(\vec{r}_{2} - \vec{r}_{2}')\delta(\vec{r}_{1} - \vec{r}_{2}), \\ &\text{where the relative-momentum operators read} \ \hat{\vec{k}} = \frac{1}{2i}\left(\vec{\nabla}_{1} - \vec{\nabla}_{2}\right), \ \hat{\vec{k}}' = \frac{1}{2i}\left(\vec{\nabla}_{1}' - \vec{\nabla}_{2}'\right). \\ &\text{*We omit the spin-orbit and tensor terms for simplicity.} \end{split}$$

JYVÄSKYLÄN YLIOPISTO

Jacek Dobaczewski



# **Regularized pseudopotentials**

We regularize delta interaction by using the Gaussian function,

$$\delta(ec{r}) = \lim_{a o 0} g_a(ec{r}) = \lim_{a o 0} rac{e^{-rac{ec{r}^2}{a^2}}}{\left(a \sqrt{\pi}
ight)^3}.$$

Then, the resulting central two-body regularized pseudopotential reads,

$$V(ec{r}_1ec{r}_2;ec{r}_1'ec{r}_2') = \sum_{i=1}^4 \hat{P}_i \hat{O}_i(ec{k},ec{k}') \delta(ec{r}_1 - ec{r}_1') \delta(ec{r}_2 - ec{r}_2') g_a(ec{r}_1 - ec{r}_2),$$

where  $\vec{k} = \frac{1}{2i}(\vec{\nabla}_1 - \vec{\nabla}_2)$  and  $\vec{k}' = \frac{1}{2i}(\vec{\nabla}_1' - \vec{\nabla}_2')$  are the standard relativemomentum operators, and the Wigner, Bartlett, Heisenberg, and Majorana terms are given by the standard spin and isospin exchange operators,  $\hat{P}_1 \equiv 1, \hat{P}_2 \equiv \hat{P}_{\sigma}, \hat{P}_3 \equiv -\hat{P}_{\tau}, \hat{P}_4 \equiv -\hat{P}_{\sigma}\hat{P}_{\tau}.$ 

To give a specific example, up to the second-order, that is, up to the next-to-leading-order (NLO) expansion, operators  $\hat{O}_i(\vec{k}, \vec{k}')$  read

$$\hat{O}_i(ec{k},ec{k}') = T_0^{(i)} + rac{1}{2} T_1^{(i)} \left( ec{k'}^{*2} + ec{k}^2 
ight) + T_2^{(i)} ec{k'}^* \cdot ec{k},$$

where  $T_k^{(i)}$  are the channel-dependent coupling constants.





YVÄSKYLÄN YLIOPISTO



# **Regularized pseudopotentials**

Let us first assume that the differential operators  $\hat{O}_i(\vec{k}, \vec{k}')$  depend only on the sum of relative momenta, that is,

$$\hat{O}_i(ec{k},ec{k}') = \hat{O}_i\left(ec{k}+ec{k}'
ight) = \hat{O}_i\left(ec{k}-ec{k}'^*
ight), ~~ ext{which requires that}~~T_2^{(i)} = -T_1^{(i)}.$$

Such particular differential operators commute with the locality deltas  $\delta(\vec{r}_1' - \vec{r}_1)\delta(\vec{r}_2' - \vec{r}_2)$ , and thus can be applied directly onto the regularized delta  $g_a(\vec{r}_1 - \vec{r}_2)$ . In such a case, the pseudopotential reduces to a simple local potential

$$V(ec{r}) = \sum\limits_{i=1}^{4} \hat{P}_i V_i(ec{r}), = \sum\limits_{i=1}^{4} \hat{P}_i \hat{O}_i(ec{k}) g_a(ec{r}),$$

Moreover, since  $\hat{O}_i(\vec{k})$  are scalar differential operators, the potentials must have forms of power series of Laplacians  $\Delta$  in  $\vec{r}$ , that is,

$$V_i(ec{r}) = \sum\limits_{n=0}^{n_{max}} V_{2n}^{(i)} \Delta^n g_a(ec{r}),$$

VÄSKYLÄN YLIOPISTO

where  $V_{2n}^{(i)}$  are the coupling constants at order 2n.



### **Regularized pseudopotentials vs. Gogny**



39, 125103 (2012) Ċ J.D, K. Bennaceur, F. Raimondi, J. Phys.

# **Regularized pseudopotentials vs. Gogny**





JYVÄSKYLÄN YLIOPISTO



# **Coupling constants of the regularized** pseudopotentials





### Order of expansion 2n





ÄSKYLÄN YLIOPISTO



# **Coupling constants of the regularized pseudopotentials in natural units**





### **Skyrme's three-body interaction**



Nuclear Physics 9 (1959) 615-634; C North-Holland Publishing Co., Amsterdam Not to be reproduced by photoprint or microfilm without written permission from the publisher

#### THE EFFECTIVE NUCLEAR POTENTIAL

#### T. H. R. SKYRME

Atomic Energy Research Establishment, Harwell, Didcot, Berks.

Received 18 October 1958

The effective interaction potential will *not* be the same as that defined in the self-consistent many-body theory (to which the variational principle is not applicable). The potential used in our analysis must contain three-body, and generally many-body, terms which describe the way in which interaction between two particles is influenced by the presence of others; the two-body terms alone should be related closely to the scattering between free nucleons.

These considerations have led to the following ansatz for the form of the effective potential:

$$T = \sum_{i < j} \sum_{i < j} t_{ij} + \sum_{i < j < k} \sum_{i < j < k} t_{ijk}$$
(2)

in which the many-body effects have been simulated by three-body terms alone, for the sake of simplicity of calculation.





JYVÄSKYLÄN YLIOPISTO



### The density dependence is born

PHYSICAL REVIEW C

VOLUME 5, NUMBER 3

MARCH 1972

#### Hartree-Fock Calculations with Skyrme's Interaction. I. Spherical Nuclei\*

D. Vautherin and D. M. Brink

For the three-body force Skyrme also assumed a zero-range force

$$v_{123}^{(3)} = t_3 \delta(\mathbf{\ddot{r}}_1 - \mathbf{\ddot{r}}_2) \delta(\mathbf{\ddot{r}}_2 - \mathbf{\ddot{r}}_3).$$
(7)

In the following we will show that for Hartree-Fock calculations of even-even nuclei, this force is equivalent to a two-body density-dependent interaction:

Volume 56B, number 3

#### PHYSICS LETTERS

others.

28 April 1975

(8)

#### SPIN SATURATION AND THE SKYRME INTERACTION $\stackrel{\text{\tiny \scale}}{\to}$

#### B.D. CHANG\*

Received 18 March 1975

Of existing variants of the Skyrme interaction, those with strong three-body terms – in particular the variant SIII that is in best accord with experiment – overbind odd-mass and odd-odd nuclei and produce unstable spin-saturated Hartree-Fock ground states in nuclear matter and in even-even light nuclei. This difficulty can be removed either by imposition of an additional stability condition or by abandoning the three-body term in favor of the two-body density-dependent interaction equivalent to it in spin-saturated HF states.









 $v_{12} = \frac{1}{6}t_3(1+P_{\sigma})\delta(\mathbf{\vec{r}}_1-\mathbf{\vec{r}}_2)\rho\left(\frac{\mathbf{\vec{r}}_1+\mathbf{\vec{r}}_2}{2}\right).$ 

Such a term provides a simple phenomenological

scribes the way in which the interaction between

representation of many-body effects, and de-

two nucleons is influenced by the presence of

### The density dependence is exploited

1.E.2

Nuclear Physics A238 (1975) 29-69; C North-Holland Publishing Co., Amsterdam

Not to be reproduced by photoprint or microfilm without written permission from the publisher

#### NUCLEAR GROUND-STATE PROPERTIES AND SELF-CONSISTENT CALCULATIONS WITH THE SKYRME INTERACTION (I). Spherical description

M. BEINER, H. FLOCARD and NGUYEN VAN GIAI

#### TABLE 5

Binding energy per particle E/A, Fermi momentum  $k_F$ , incompressibility coefficient K, effective mass ratio  $m^*/m$  and symmetry coefficients  $\varepsilon_1$  and  $\varepsilon_2$  [see eq. (17)] in nuclear matter calculated with the interactions SII to SVI

	t <sub>3</sub> (MeV fm <sup>6</sup> )	<i>E/A</i> (MeV)	k <sub>F</sub> (fm <sup>-1</sup> )	K (MeV)	<b>m*</b> /m	ε <sub>i</sub> (MeV)	ε <sub>2</sub> (MeV)
SVI	17000	-15.77	1.29	364	0.95	26.89	0.67
SIII	14000	-15.87	1.29	356	0.76	28.16	0.83
SII	9331	-16.00	1.30	342	0.58	34.2	1.10
SIV	5000	-15.98	1.31	325	0.47	31.22	1.37
SV	0	-16.06	1.32	306	0.38	32.72	1.70

The interactions have been ordered according to the decreasing values of the parameter  $t_3$ .









# The density dependence causes havoc

Particle-number projection impossible Strong self interaction present



FIG. 11. (Color online) Deformation energy  $E(\beta)$  as a function of quadrupole deformation  $\beta$  calculated for <sup>32</sup>Mg with the SIII force and volume pairing interaction. Results of the PAV HFB+LN calculations (squares and triangles) are compared with the VAP PNP results (dots). The standard HFB result is shown by open triangles.

J.D. et al., Phys. Rev. C 76, 054315 (2007)



D. Tarpanov. et al., to be published





YVÄSKYLÄN YLIOPISTO



# First density-independent finite-range functional generator at a=0.8fm

#### **Results with SV:**

$ ho_{ m sat}$	E/A	$K_\infty$	J	L	$K_{ m sym}$	
$0.1551 { m ~fm^{-3}}$	$-16.05~{\rm MeV}$	$305.7 \ \mathrm{MeV}$	$32.82 { m MeV}$	96.09 MeV	$24.17~{\rm MeV}$	

Nuc.	<sup>40</sup> Ca	<sup>48</sup> Ca	<sup>56</sup> Ni	<sup>78</sup> Ni	<sup>100</sup> Sn	$^{132}Sn$	<sup>208</sup> Pb
$E^{\exp}$	-342.050	-415.998	-483.991	-641.780	-824.921	-1102.827	-1636.350
$E^{\text{calc}}$	-342.985	-418.177	-472.783	-650.148	-817.793	-1109.998	-1636.463
diff.	-0.935	-2.179	11.208	-8.368	7.128	-7.171	-0.113

#### Results with a = 0.8 fm:

$ ho_{ m sat}$	E/A	$K_\infty$	J	L	$K_{ m sym}$	
$0.1600 \ {\rm fm}^{-3}$	$-16.00 { m MeV}$	$230.0  \mathrm{MeV}$	$32.00 { m MeV}$	$100.2 \ \mathrm{MeV}$	$83.26 { m MeV}$	

Nuc.	<sup>40</sup> Ca	<sup>48</sup> Ca	<sup>56</sup> Ni	<sup>78</sup> Ni	<sup>100</sup> Sn	$^{132}Sn$	<sup>208</sup> Pb
$E^{ m exp}$	-342.050	-415.998	-483.991	-641.780	-824.921	-1102.827	-1636.350
$E_{10}^{ m calc}$	-341.876	-422.960	-480.475	-644.712	-821.079	-1101.619	-1622.441
diff.	-0.355	-8.017	2.031	-4.495	0.941	-2.080	6.404





JYVÄSKYLÄN YLIOPISTO



## Masses of doubly magic nuclei





# Conclusions

- 1. We introduced a new class of energy density functionals that are based on regularized pseudopotentials. They allow for constructing density-independent functional generators.
- 2. In our opinion, future prospects for using the proposed regularized (pseudo)potentials are high.
  - a. They may present better convergence properties than similar expansions based on the zero-range interactions.
  - b. They allow for convergent summations of contributions from high single-particle momenta,
  - c. They allow for formulating a consistent expansion in terms of the orders of derivatives, with the convergence properties gauged against the regularization scale.
  - d. They allow for consistent beyond-mean field calculations.
- 3. The regularized pseudopotentials give us a possibility of building an order-by-order correctible theory.



YVÄSKYLÄN YLIOPISTO



# Thank you





JYVÄSKYLÄN YLIOPISTO



# **Rayleigh-Ritz Variational Method**

$$egin{aligned} \hat{H}|\Psi_i
angle &= E_i|\Psi_i
angle \ & \Downarrow \ & |\Psi
angle &= a_0|\Psi_0
angle + a_1|\Psi_1
angle + a_2|\Psi_2
angle + \ldots \ & \langle\Psi|\hat{H}|\Psi
angle &= E_0|a_0|^2 + E_1|a_1|^2 + E_2|a_2|^2 + \ldots \ & \Downarrow \ & \Downarrow \ & \min_{|\Psi
angle} \langle\Psi|\hat{H}|\Psi
angle &= E_0 & \Leftarrow ext{Rayleigh-Ritz} \end{aligned}$$

JYVÄSKYLÄN YLIOPISTO



r



### Energy density functional up to N<sup>3</sup>LO

Local (primary) densities are defined by four quantum numbers nLvJ as

$$ho_{nLvJ}^t(ec{r}) = \left\{ [K_{nL} 
ho_v^t(ec{r}, ec{r}')]_J 
ight\}_{ec{r}'=ec{r}},$$

where the *n*th-order and rank-*L* relative derivative operators  $K_{nL}$  act on the scalar (v = 0) or vector (v = 1) isoscalar (t = 0) or isovector (t = 1) nonlocal densities.

We act on each of the local primary densities with *m*th-order and rank-*I* derivative operator  $D_{mI}$ , and then couple ranks *I* and *J* to the total rank *J'*, which gives the local secondary densities,  $[D_{mI}\rho_{nLvJ}^t(\vec{r})]_{J'}$ . From primary and secondary densities we build terms of the EDF:

$$T_{mI,nLvJ}^{n'L'v'J',t}(\vec{r}) = [\rho_{n'L'v'J'}^t(\vec{r})[D_{mI}\rho_{nLvJ}^t(\vec{r})]_{J'}]_0,$$

Then, the total energy density reads

$$\mathcal{H}(\vec{r}) = \sum_{\substack{n'L'v'J',t\\mI,nLvJ,J'}} C_{mI,nLvJ}^{n'L'v'J',t} T_{mI,nLvJ}^{n'L'v'J',t}(\vec{r}),$$

where  $C_{mI,nLvJ}^{n'L'v'J',t}$  are coupling constants and the summation again runs over all allowed indices.

ZÄSKYLÄN YLIOPISTO

Jacek Dobaczewski



# **Energy density functional up to N<sup>3</sup>LO** Numbers of local densities



#### Numbers terms in the EDF

Multiply by a		order	<b>T-even</b>	T-odd	total	Galilean	Gauge
factor of 2 for						invariant	invariant
· 1 1	6	0	1	1	2	2	2
isoscalar and		2	6	6	12	7	7
isovector	$\rightarrow$	4	22	23	45	15	6
terms		6	64	65	129	26	6
	′	N <sup>3</sup> LO	93	95	188	50	21





# **Convergence of the DME**

The success and convergence of the DME expansions relies on the fact that the finite-range nuclear effective interactions (Gmatrix, Gogny, M3Y,...) are very short-range as compared to the spatial variations of nuclear densities. The quasi-local (gradient) expansion in nuclei works!

DME for the Gogny direct energy

DME for the Gogny exchange energy



# Pseudopotentials vs. energy density functional

Number of terms in the pseudopotential								
Galilean	2	7	15	26	50			
Gauge	2	7	6	6	21			

At any order and symmetry, the number of terms in the pseudopotential is exactly equal to the number of the EDF terms <u>for each isospin</u>. Therefore, there are <u>always</u> twice as many EDF terms as there are pseudopotential terms

For the fourth-order gauge-invariant pseudopotential, the EDF isvector terms can be expressed as linear combinations of the isoscaler terms as:

$C_{mI,nLvJ}^{n'L'v'J',1}$	= A(a	$C^{2202,0}_{00,2202} +$	$bC_{00,2212}^{2212,0} +$	$cC_{00,4211}^{0011,0}$ ·	$+  dC^{0000,0}_{40,0000}$	$+ eC_{40,00}^{0011}$	$_{011}^{,0}$ +	$fC_{42,001}^{0011,0}$
	A	a	b	с	d	e	f	
$C_{40,0000}^{0000,1}$	$\frac{1}{120}$	$-6\sqrt{15}$	$-18\sqrt{15}$	$-21\sqrt{5}$	$-40\sqrt{3}$	0	0	
$C_{40,0011}^{0011,1}$	$\frac{1}{120}$	$-18\sqrt{5}$	$18\sqrt{5}$	$7\sqrt{15}$	0	$-40\sqrt{3}$	0	
$C_{42,0011}^{0011,1}$	$-\frac{1}{\sqrt{3}}$	0	0	1	0	0	1	
$C^{2202,1}_{00,2202}$	1	$-3\sqrt{3}$	0	0	$-4\sqrt{15}$	$-12\sqrt{5}$	0	
$C_{00,4211}^{0011,1}$	$-\frac{1}{\sqrt{2}}$	0	0	1	0	0	4	
$C^{2212,1}_{00,2212}$	$\frac{1}{9}$	0	$-3\sqrt{3}$	0	$-4\sqrt{15}$	$4\sqrt{5}$	14	

Jacek Dobaczewski



JYVÄSKYLÄN YLIOPISTO



### **Continuity equation**

Within the Kohn-Sham approach, the total energy is the sum of the kinetic and potential-energy terms,

 $E\{\rho\} = E_k\{\rho\} + E_p\{\rho\},\$ 

Let us now assume that the potential energy is invariant with respect to a unitary transformation of the density matrix,  $U = \exp(i\eta G)$ ,

 $E_p\{
ho\} = E_p\{U
ho U^+\}, \implies {
m Tr}\Gamma[G,
ho] \equiv {
m Tr}G[\Gamma,
ho] = 0,$ 

which allows us to derive the equation of motion for the average value of  $\langle G \rangle = \text{Tr} G \rho$ .

$$i\hbar rac{\mathrm{d}}{\mathrm{d}t} \langle G 
angle = i\hbar \mathrm{Tr} G rac{\mathrm{d}}{\mathrm{d}t} 
ho = \mathrm{Tr} G[h, 
ho] = \mathrm{Tr} G[T, 
ho],$$

that is, the time evolution of  $\langle G \rangle$  is governed solely by the kinetic term of the mean-field Hamiltonian.

The CE now results from specifying  $\eta G$  to the local gauge transformation, that is,  $\psi'_{\alpha}(r\sigma\tau) \equiv (U\psi_{\alpha})(r\sigma\tau) = e^{i\gamma(r)}\psi_{\alpha}(r\sigma\tau)$ , which gives,

$$rac{\mathrm{d}}{\mathrm{d}t}
ho_{00}(r,t)=-rac{\hbar}{m}
abla\cdot j_{00}(r,t).$$

JYVÄSKYLÄN YLIOPISTO





# 

- **1) Exact:** Minimization of E(Q) gives the exact E and exact Q
- Impractical: Derivation of E(Q) requires the full variation δ (bigger effort than to find the exact ground state)
- **3) Inspirational:** Can we build useful models E'(Q) of the exact E(Q)?
- **4) Experiment-driven:** E'(Q) works better or worse depending on the physical input used to build it.



JYVÄSKYLÄN YLIOPISTO



#### **Pseudopotentials**

In the central-like form, the pseudopotential is a sum of terms,

$$\hat{V} = \sum_{\tilde{n}'\tilde{L}'\tilde{n}\tilde{L}, v_{12}S} C_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'} \hat{V}_{\tilde{n}\tilde{L}, v_{12}S}^{\tilde{n}'\tilde{L}'}.$$

Each term in the sum is accompanied by the corresponding strength parameter  $C_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'}$ , and explicitly reads,

$$\begin{split} \hat{V}_{\tilde{n}\tilde{L},v_{12}S}^{\tilde{n}'\tilde{L}'} &= \quad \frac{1}{2} i^{v_{12}} \left( \left[ \left[ K_{\tilde{n}'\tilde{L}'}'K_{\tilde{n}\tilde{L}} \right]_{S} \hat{S}_{v_{12}S} \right]_{0} + (-1)^{v_{12}+S} \left[ \left[ K_{\tilde{n}\tilde{L}}'K_{\tilde{n}'\tilde{L}'} \right]_{S} \hat{S}_{v_{12}S} \right]_{0} \right) \\ &\times \left( 1 - \hat{P}^{M}\hat{P}^{\sigma}\hat{P}^{\tau} \right) \hat{\delta}_{12}(r_{1}'r_{2}';r_{1}r_{2}). \end{split}$$

 $K_{\tilde{n}\tilde{L}}$  are the spherical tensor derivatives of order  $\tilde{n}$  and rank  $\tilde{L}$  are built of  $k = (\nabla_1 - \nabla_2)/2i$ , The two-body spin operators  $\hat{S}_{v_{12}S}$  are defined as,

$$\hat{S}_{v_{12}S} = \left(1 - rac{1}{2}\delta_{v_1,v_2}
ight) \left([\sigma^{(1)}_{v_1}\sigma^{(2)}_{v_2}]_S + [\sigma^{(1)}_{v_2}\sigma^{(2)}_{v_1}]_S
ight),$$

where  $v_{12} = v_1 + v_2$  and  $\sigma_{v\mu}^{(i)}$  are the spherical-tensor components of the rank-v Pauli matrices. The Dirac delta function,

$$\hat{\delta}_{12}(\vec{r}_1'\vec{r}_2',\vec{r}_1\vec{r}_2) = \delta(\vec{r}_1'-\vec{r}_1)\delta(\vec{r}_2'-\vec{r}_2)\delta(\vec{r}_1-\vec{r}_2),$$

ensures the locality and zero-range character of the pseudopotential.

JYVÄSKYLÄN YLIOPISTO



# **Regularized pseudopotentials**

Below we determine coupling constants  $V_{2n}^{(i)}$  in Eq. (??) by requiring that the lowest moments of the regularized and Gogny potentials are equal, that is,

$$M_{2m}^{(i)}\equiv\int r^{2m}G_i(r)\mathrm{d}^3r=\int r^{2m}V_i(r)\mathrm{d}^3r,$$

for  $m = 0, 1, ..., n_{max}$ . This conditions gives the coupling constants of the regularized potential in simple analytical forms,

$$\begin{split} V_{2n}^{(i)} &= \sum_{m=0}^{n} \left( -\frac{a^2}{4} \right)^{n-m} \frac{M_{2m}^{(i)}}{(n-m)!(2m+1)!} \\ &= \frac{1}{4^n n!} \sum_{k=1,2} G_k^{(i)} \left( a_k^2 - a^2 \right)^n, \end{split}$$

where  $G_k^{(i)}$  and  $a_k$  are the parameters of the Gogny interaction.

/ÄSKYLÄN V





### **Regularized pseudopotentials vs. Gogny**







SKVLÄN YLIOPISTO



32/21

39, 125103 (2012)

Ċ

Raimondi, J. Phys.

Ē

J.D, K. Bennaceur,

# **Regularized pseudopotentials vs. Gogny**



Figure 3. The same as in figure 2, but for the deviations of binding energies scaled by the numbers of particles,  $\Delta b = \Delta B/A$ , and those of radii scaled by the nuclear sizes,  $\Delta r = \Delta R/A^{1/3}$ . Note that the N<sup>2</sup>LO results almost perfectly hide behind those obtained at N<sup>3</sup>LO.

Jacek Dobaczewski





















