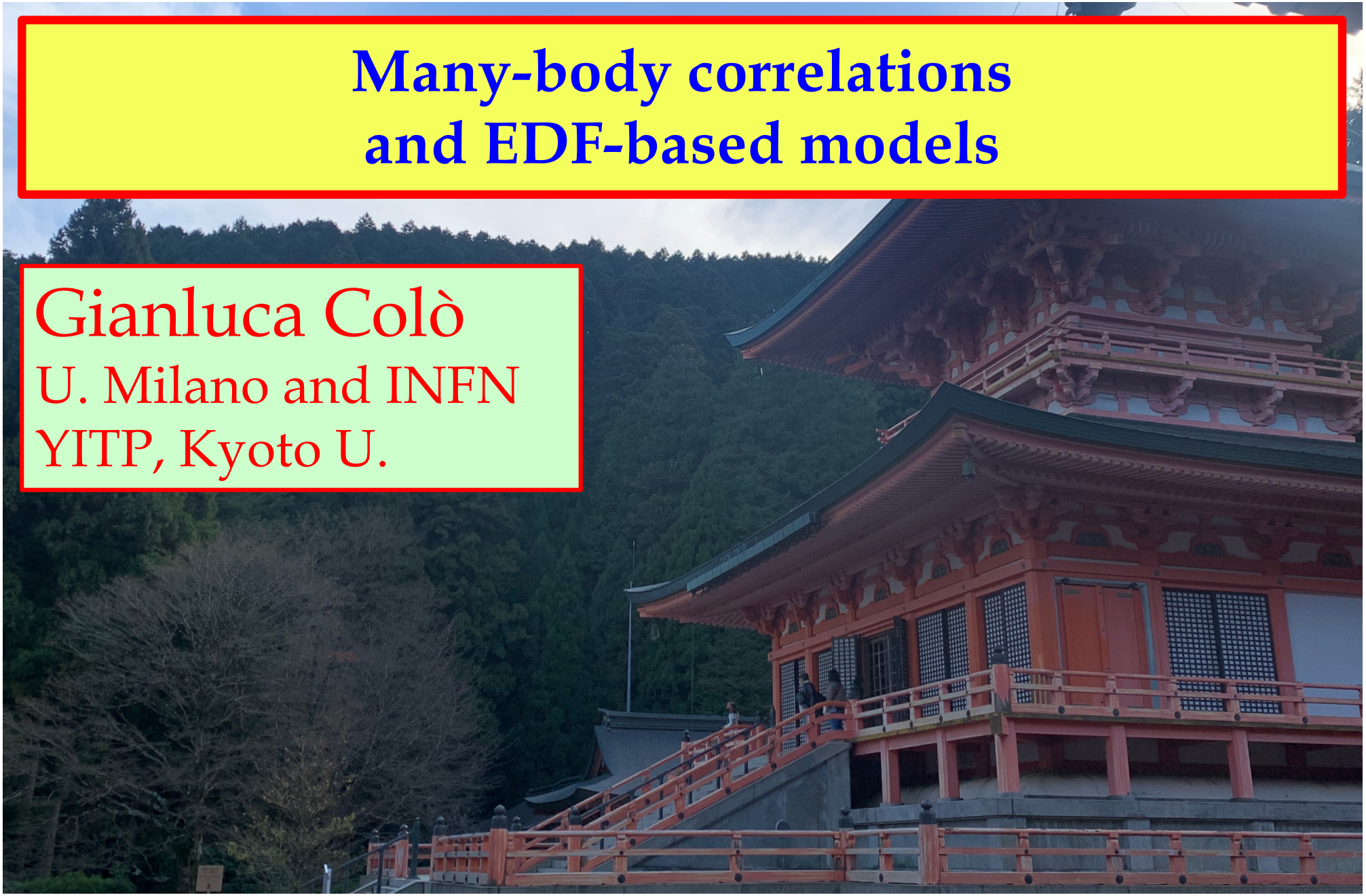
Many-body correlations and EDF-based models



Gianluca Colò
U. Milano and INFN
YITP, Kyoto U.

Kyoto, 9 Dec. 2022

Outline of the talk

- Recap of nuclear EDFs (very short, cf. previous talks in this workshop)
- New strategies to build EDFs
- Many-body correlations ("PVC vs GW")

Nuclear EDF (cf. N. Hinohara, K. Sekizawa ...)

$$E = \int d^3r \ \left[\mathcal{E}^{\rm kin} + \mathcal{E}^{\rm Skyrme} + \mathcal{E}^{\rm pairing} + \mathcal{E}^{\rm Coulomb}\right]$$

$$\mathcal{E}^{\rm Skyrme} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

Labels related to p, n were omitted for simplicity.

The quadratic form ensures the respect of the symmetries.

In principle, all coupling constants could be functions of the densities.

Coulomb: known. Exchange is often approximated (e.g.: Slater approximation).

1. In the case of Coulomb EDFs, the underlying interaction is known, and the Hartree term is well-defined so that the "functional" is defined by the choice for $E_{\rm xc}$.

HF and KS-DFT are clearly distinguished for Coulomb systems.

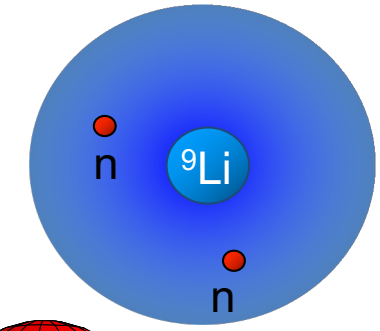
2. In the nuclear case, so far, all EDFs are based on an ansatz for the form of $\mathcal{E}$, and a parameter fit. There is no underlying "fundamental force", so that Hartree, exchange and correlations are mixed up in the terms of the EDF.

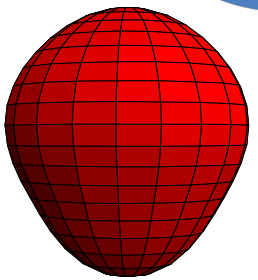
HF with effective forces and KS-DFT are connected.

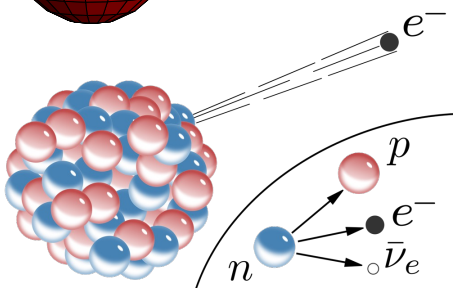
GC, *Nuclear DFT* in:
Tanihata, I., Toki, H., Kajino, T. (eds)
Handbook of Nuclear Physics, Springer, Singapore, 2022.

Status of nuclear DFT (very brief...)

- Error on **masses** of the order of 1 MeV.
- Predictions of **drip lines** and **super heavy** nuclei.
- Trends of **charge radii and deformations** fairly well reproduced.
- Advanced (multi-reference) techniques based on **symmetry restoration.**
- **Giant resonances, charge-exchange states and β-decay.**
- Current interest in **large amplitude motion, reactions** etc.







Many observables (pseudo-observables)

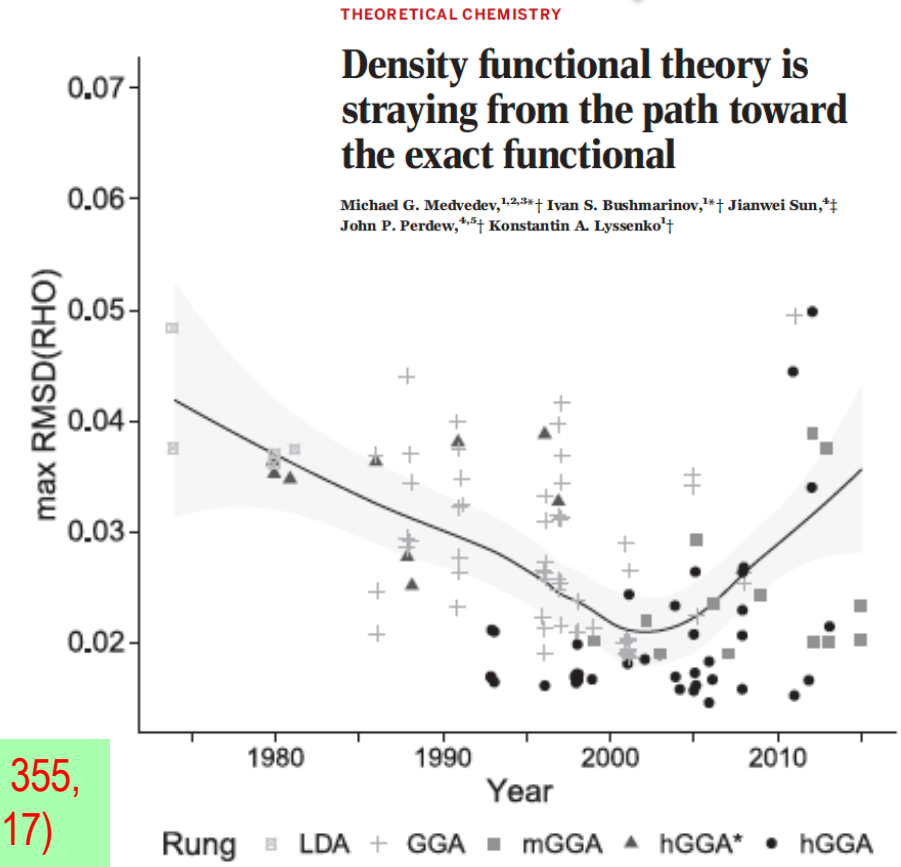
Many PARAMETER SETS for EDFs

NEW TECHNIQUES

→ **Risk of overfitting**

↓

Keep an eye on DFT from *ab initio*



Science 355, 49 (2017)

- New strategies to build EDFs

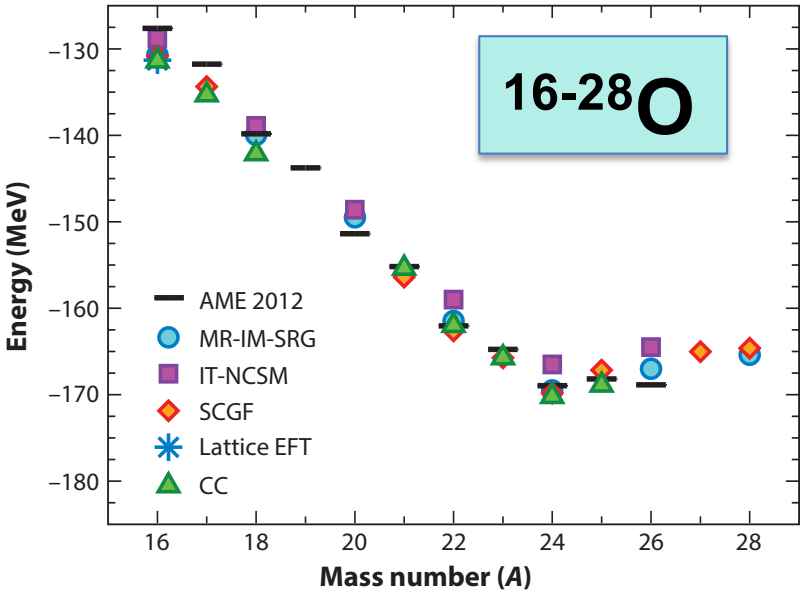
Several possibilities

- Bayesian inference, machine learning...
- Building the EDFs from *ab initio*.
- Reverse engineering: deduce EDFs from reliable energies/densities (i.e. the inverse KS problem).

Ab initio: still behind respect to Coulomb

Ab initio aims at solving the nuclear many-body problem using a **realistic Hamiltonian** and a **many-body method that is, in principle, exact** (or whose uncertainty can be quantified).

H is a larger source of uncertainties than the MB method.



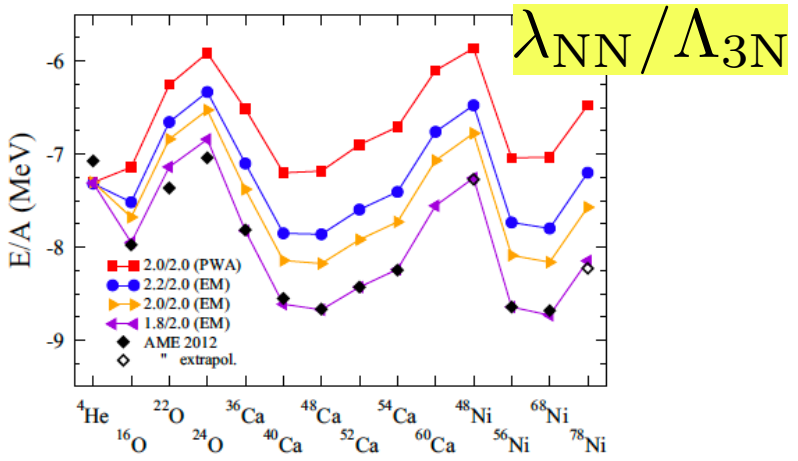


FIG. 5. Systematics of the energy per nucleon E/A of closed-shell nuclei from ^{4}He to ^{78}Ni calculated with the IM-SRG for the four Hamiltonians considered. The results are compared against experimental ground-state energies from the AME 2012 [40] (extrapolated for ^{48,78}Ni).

J. Simonis et al., Phys. Rev. C 96, 014303 (2017)

PHYSICAL REVIEW C **104**, 024315 (2021)

Nuclear energy density functionals grounded in *ab initio* calculations

F. Marino,[1,2,*] C. Barbieri,[1,2] A. Carbone,[3] G. Colò,[1,2] A. Lovato,[4,5] F. Pederiva,[6,5] X. Roca-Maza,[1,2] and E. Vigezzi[2]

[1]*Dipartimento di Fisica "Aldo Pontremoli," Università degli Studi di Milano, 20133 Milano, Italy*
[2]*Istituto Nazionale di Fisica Nucleare, Sezione di Milano, 20133 Milano, Italy*
[3]*Istituto Nazionale di Fisica Nucleare–CNAF, Viale Carlo Berti Pichat 6/2, 40127 Bologna, Italy*
[4]*Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
[5]*Istituto Nazionale di Fisica Nucleare–Trento Institute of Fundamental Physics and Applications, 38123 Trento, Italy*
[6]*Dipartimento di Fisica, University of Trento, via Sommarive 14, 38123 Povo, Trento, Italy*

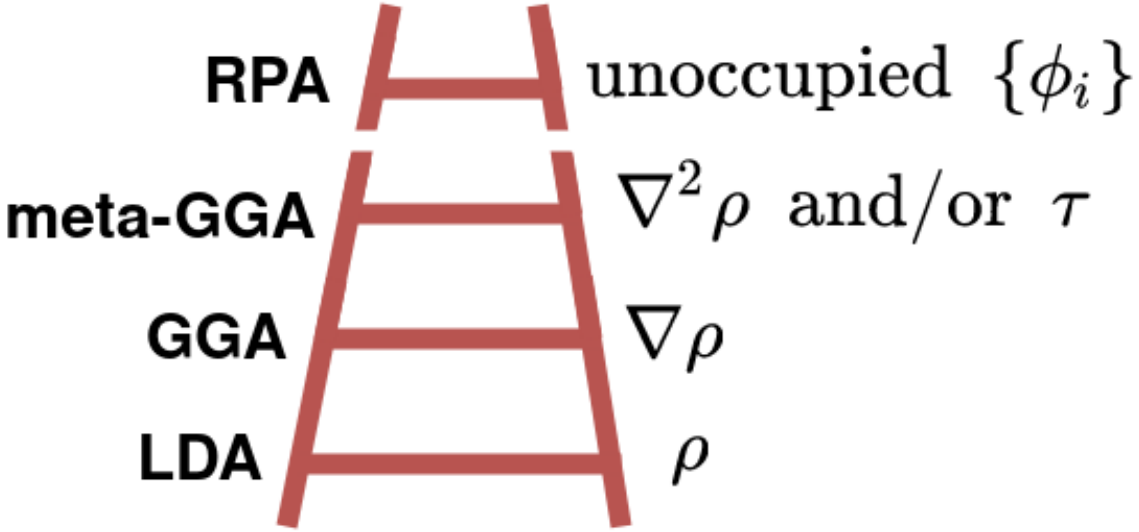
Quantum Monte Carlo (QMC)

Self-consistent Green's Function (SCGF) method

Our systematic ladder of approximations

Our strategy based on the **Jacob's ladder** of electronic DFT.

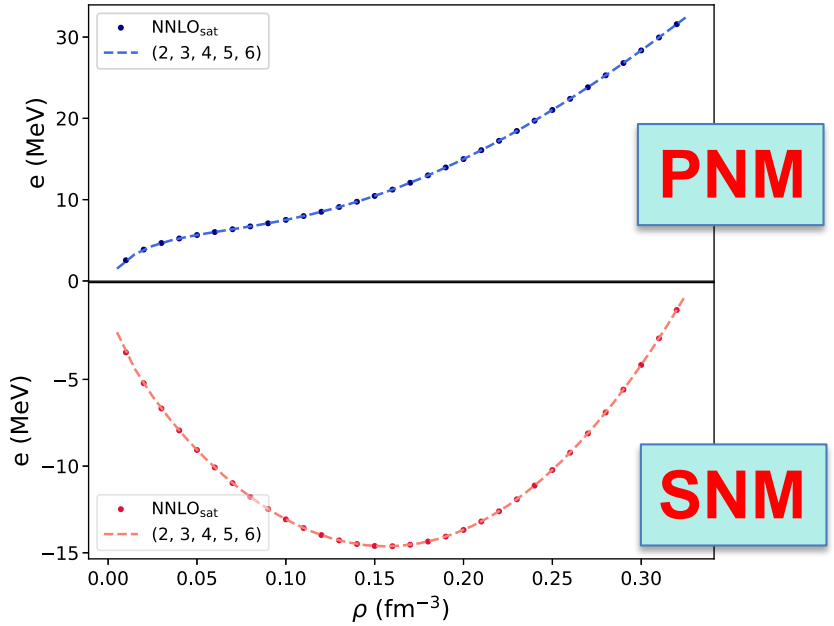
J. Perdew, K. Schmidt, AIP Conf. Proc. 577, 1 (2001).



- **Follow a step-by-step approach**
- **Use *ab initio* simulations of model systems as a constraint**

Local Density Approximation (LDA)

We start from the Equation of State (EoS) of nuclear matter.



$$e = \frac{E}{A} = \frac{\mathcal{E}}{\rho}$$

Within LDA, the energy functional is the same as in uniform matter.

We apply it to finite systems as if their local density were uniform.

$$E_{\rm pot} = \int d^3r \ \rho(\vec{r}) e[\rho]$$

The Equation of State (EoS)

$$\rho = \rho_n + \rho_p$$

$$\beta = \frac{\rho_n - \rho_p}{\rho}$$

SCGF with NNLO$_{sat}$

QMC with AV4'

We parametrise the potential part of the EoS.

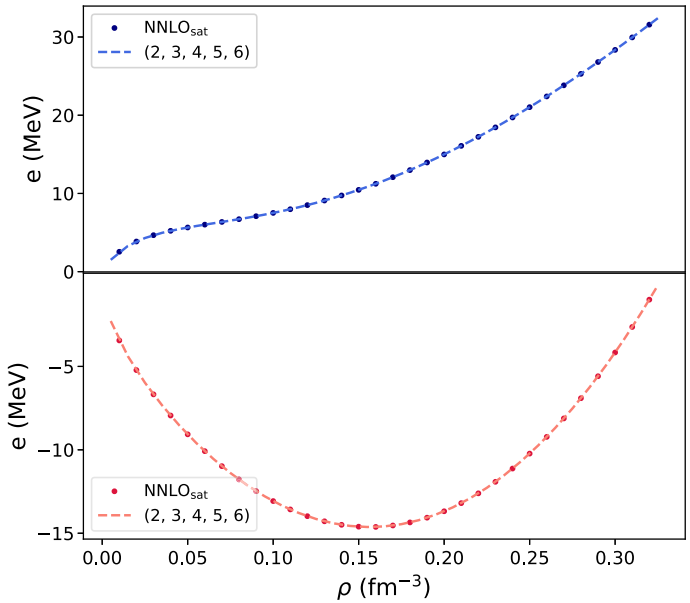
1. v is quadratic in β
2. v is a polynomial in k_F

$$v(\rho, \beta) = \sum_{\gamma} \left(c_{\gamma,0} + \beta^2 c_{\gamma,1}\right) \rho^{\gamma} \qquad \gamma = \frac{n}{3}$$

3. The optimal set of powers is chosen by model selection

EoS with different Hamiltonians

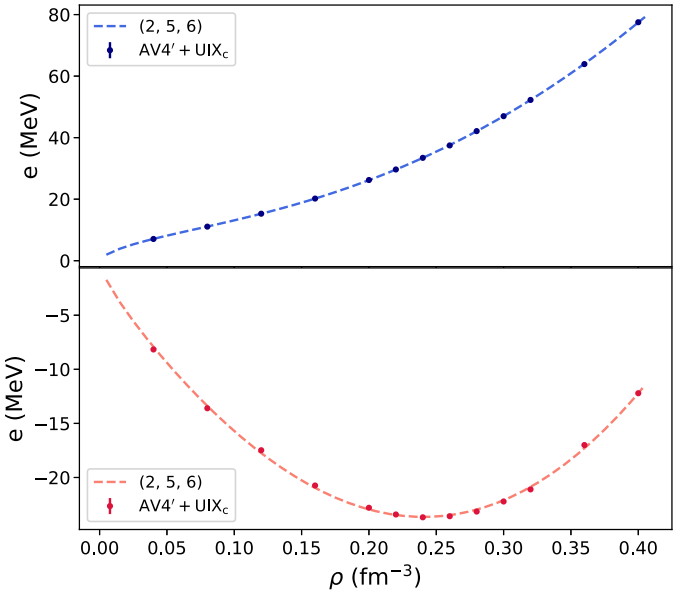
NNLO$_{sat}$



PNM

SNM

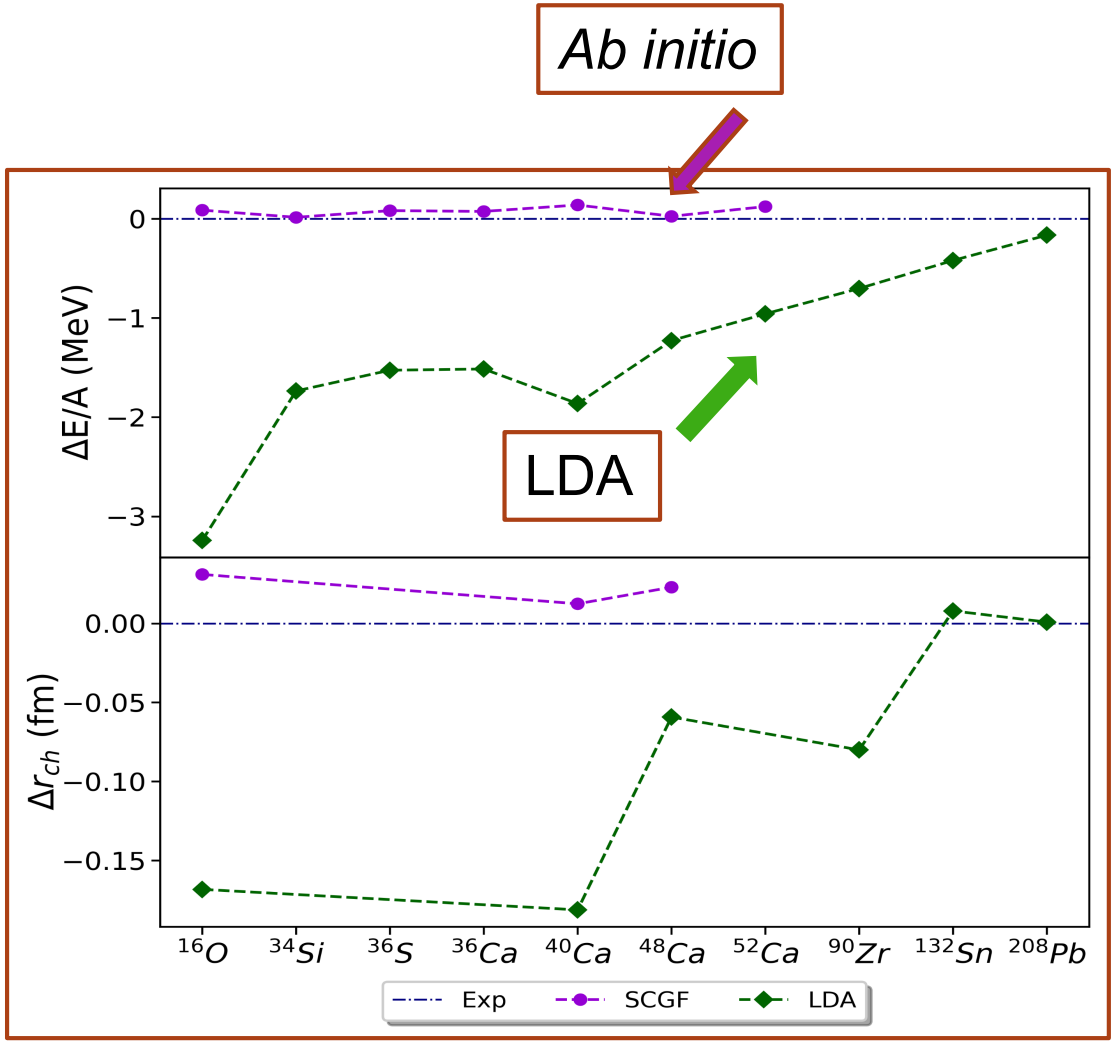
Av4'



$$\gamma = \frac{2}{3}, 1, \frac{4}{3}, \frac{5}{3}, 2$$

$$\gamma = \frac{2}{3}, \frac{5}{3}, 2$$

Results: NNLO$_{sat}$



Difference with respect to experiment for

E/A (upper panel)

r_{ch} (lower panel)

Encouraging results in heavy nuclei (^{132}Sn, ^{208}Pb)

Something still missing

Towards the gradient approximation

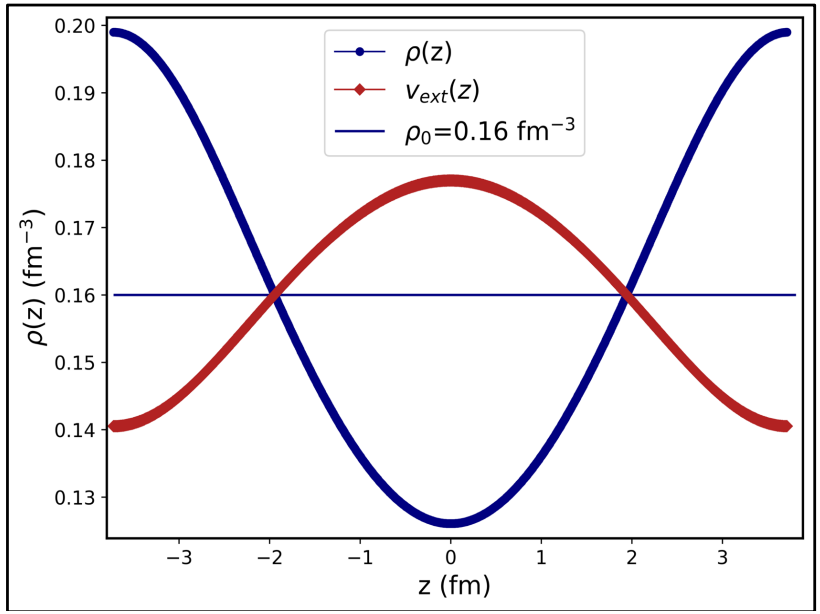
$$\mathcal{E}^{\text{Skyrme}} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

LDA

Nuclei are finite systems and the dependence of the EDF on $\nabla\varrho$, τ and J is mandatory. These quantities vanish in static uniform matter.

How can *ab initio* inform us about this dependence?

Uniform matter perturbed by a (weak) potential



Perturbed nuclear matter (I)

Add a **weak external potential** of the type: $v_{\rm ext} = 2v_q cos(\vec{q}\cdot\vec{r})$

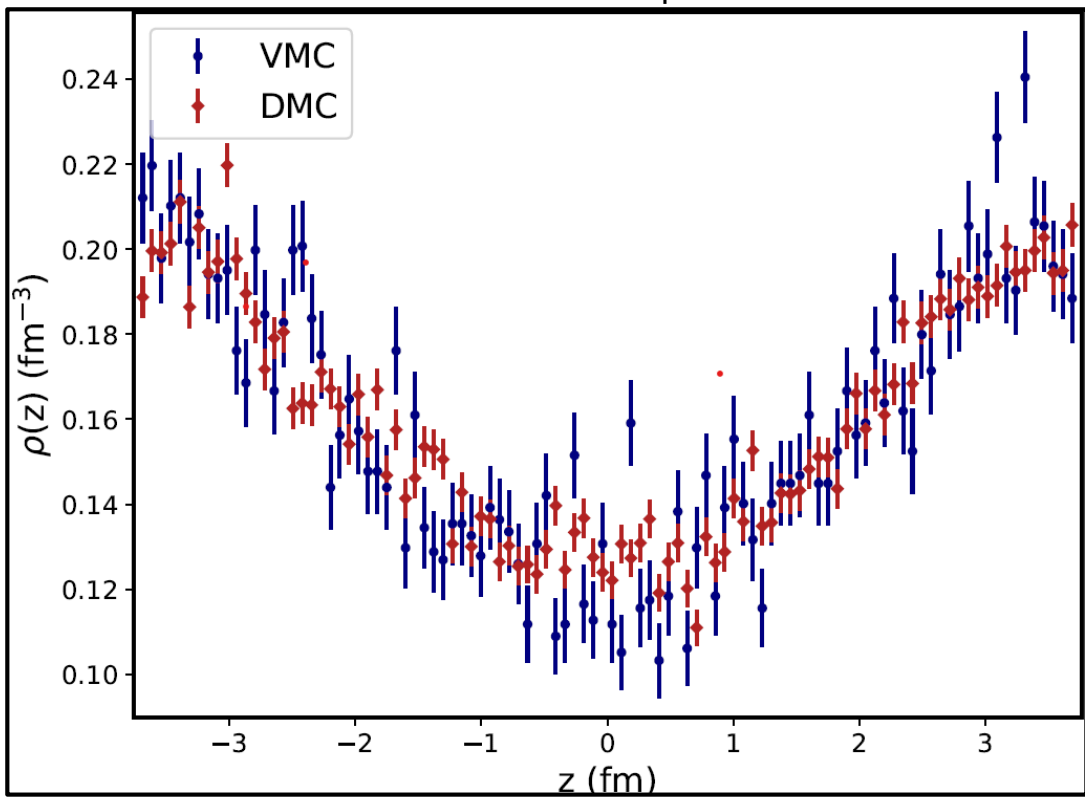
In linear response:

$$\delta\rho(\vec{r}) = 2\chi(q)v_q cos(\vec{q}\cdot\vec{r})$$

$$\delta e = \frac{\chi(q)}{\rho_0} v_q^2$$

Potential along the z axis.

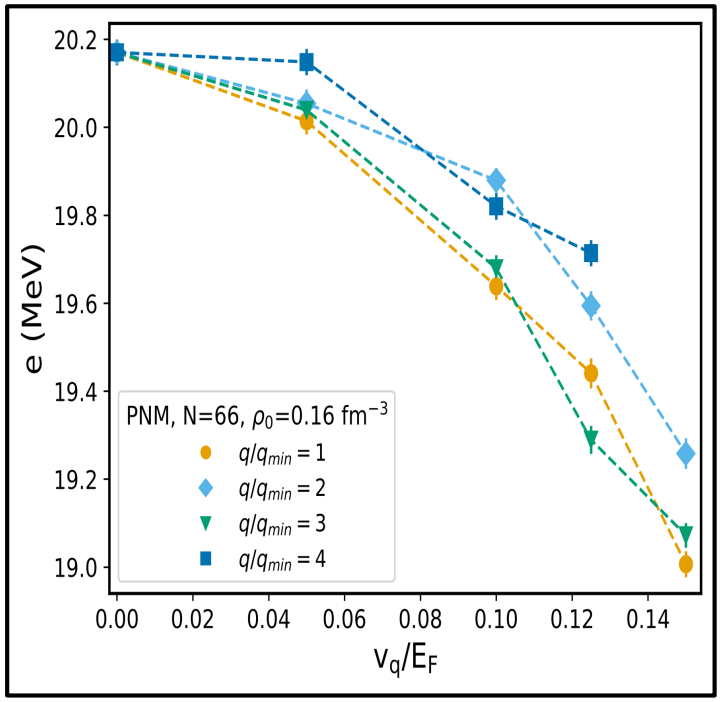
PNM, N=66, $q/q_{min}=1$, $v_q/E_F = 0.1$



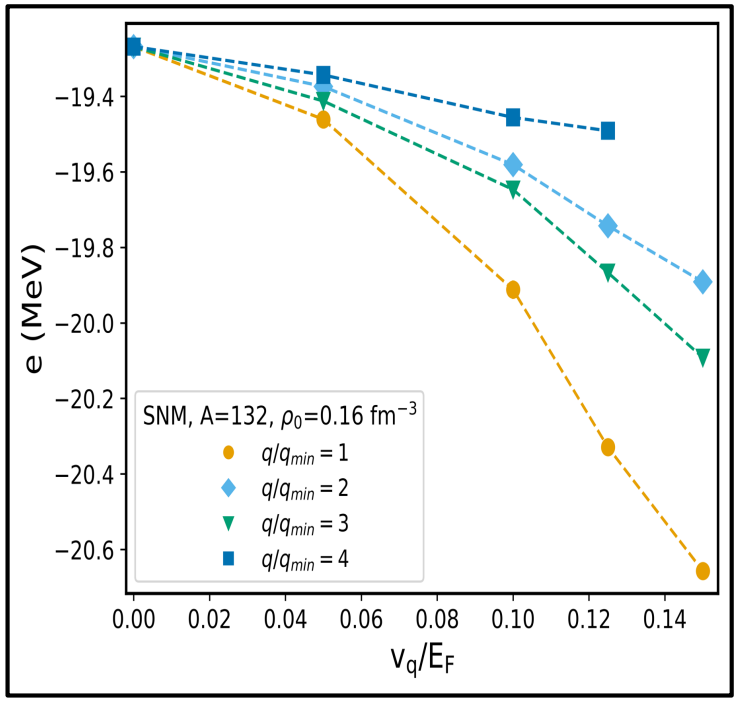
Perturbed nuclear matter (II)

Perturbing the system gives access to: $C^{\rho\tau}$ $C^{(\nabla\rho)^2}$ $C^{\rho\vec{\nabla}\cdot\vec{J}}$

Pure neutron matter



Symmetric nuclear matter



WORK IN PROGRESS

The inverse Kohn-Sham problem

Direct problem

$$F[\rho] \rightarrow v[\rho] \rightarrow \rho$$

Inverse problem

$$\rho \rightarrow v[\rho] \rightarrow F[\rho]$$

Y. Wang and R.G. Parr, Phys. Rev. A47, R1591 (1993).

R. Van Leeuwen and E.J. Baerends, Phys. Rev. A49, 2421 (1994).

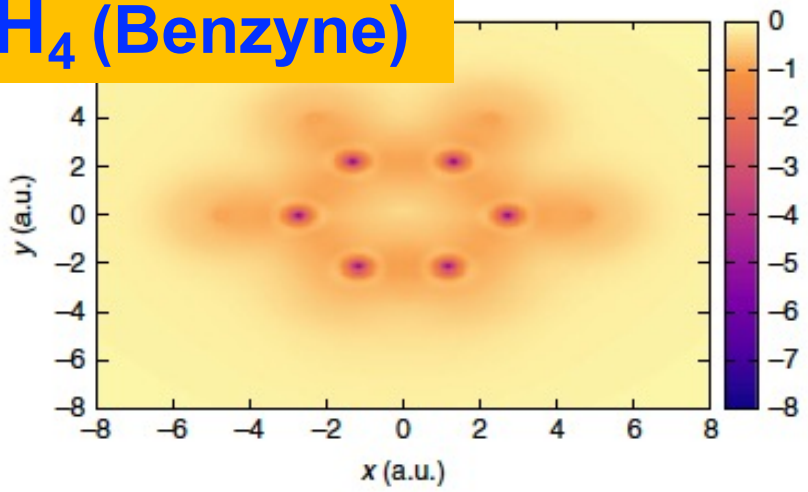
D.S. Jensen and A. Wassermann, Int. J. Quant. Chem. 118, e25425 (2018).

B. Kanungo, P.M. Zimmermann, V. Gavini, Nature Communications 10, 4497 (2019).

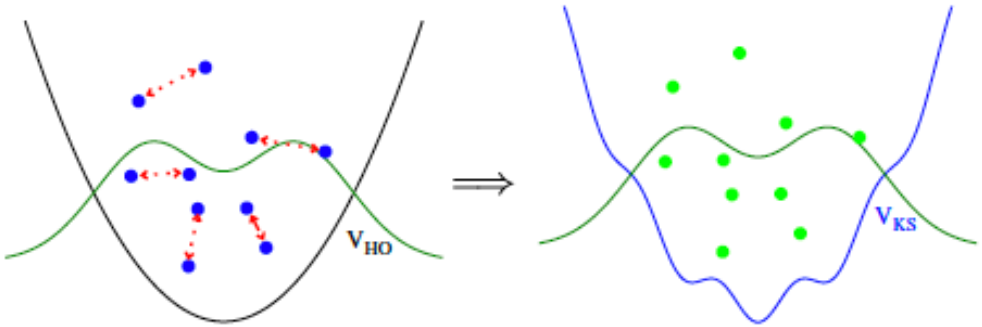
Some attempts have been made in the case of electronic systems, but not yet for atomic nuclei.

Input: target density $\tilde{\rho}(\vec{r})$

C_6H_4 (Benzyne)



The constrained variational (CV) method



In the Kohn-Sham spirit, the system at hand is assumed to be equivalent to a **non-interacting system with the same density** $\Longrightarrow$ min. of the kinetic energy T

$$J = T_s\left[\{\phi_i\}\right] + \int d^3r\; U(\vec{r})\rho(\vec{r}) - \sum_{i=1}^{N_{\rm orb}} \sum_{j=1}^{i} \epsilon_{ij} \int d^3r\; \phi_i^*(\vec{r})\phi_j(\vec{r}).$$

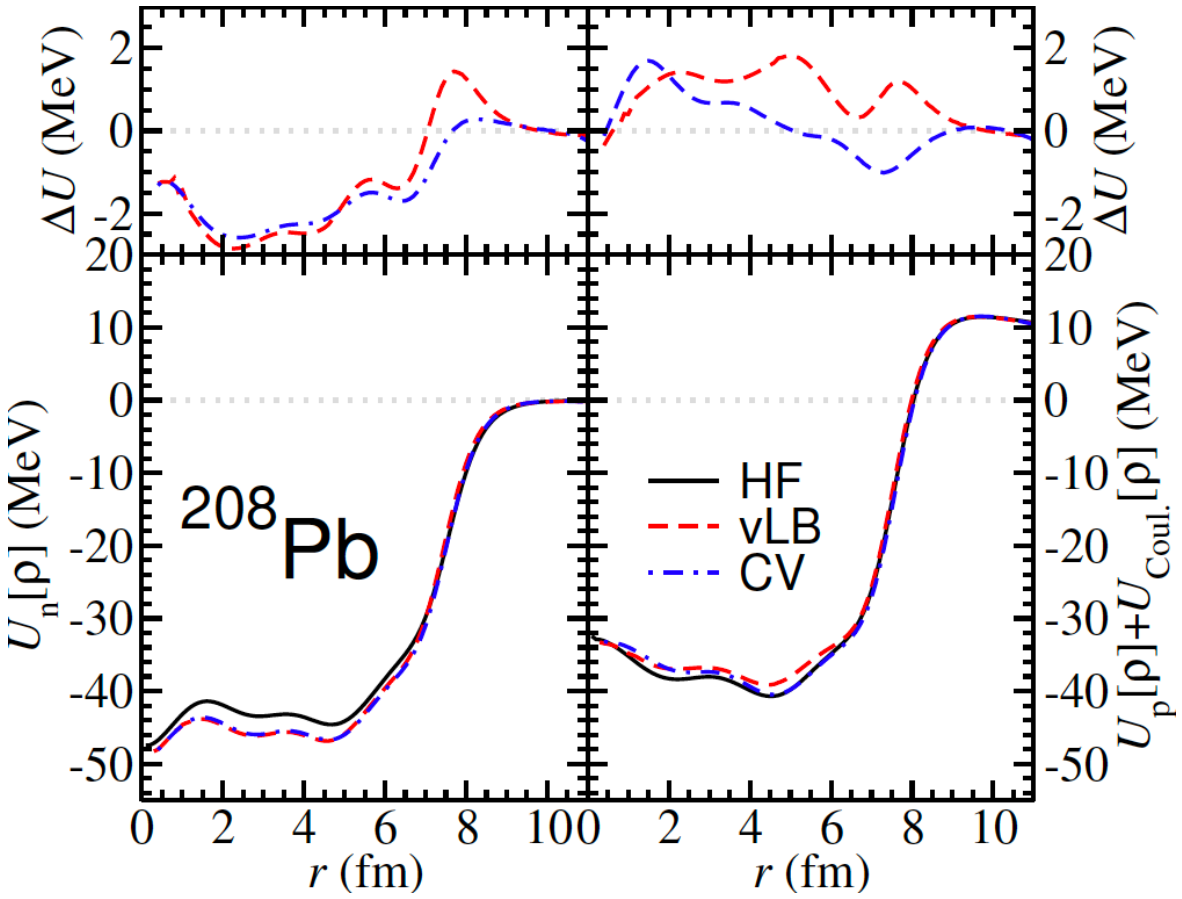
Constraints for: reproduction of target density plus orthonormality of the orbitals

$$\delta J = 0$$

The method is general/unbiased.

It relies on the IPOPT library

Test: reconstruction of SkX effective potential



SkX has an effective mass close to 1 (within ≈ 5%)

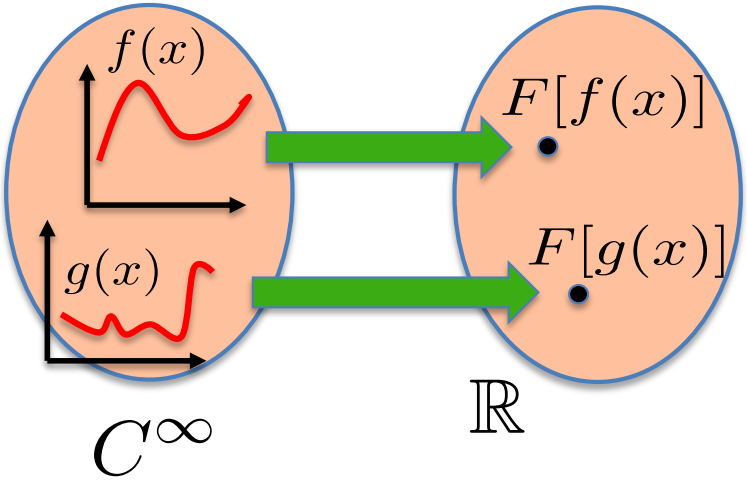
Still, **"errors"** are also associated with the fact that the problem is not well defined according to Hadamard's definition.

Coulomb tail is fairly well extracted!

How to deduce the EDF?

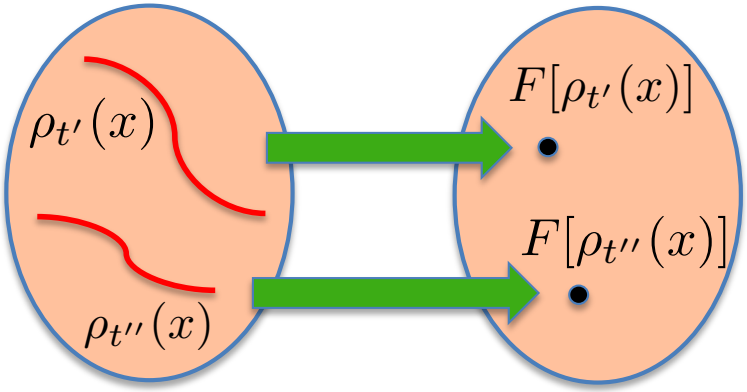
$$v[\rho] = \frac{\delta F}{\delta \rho}$$

Some kind of **functional integration** is called for.



A **line integration formula** has been proposed by Van Leeuwen and Baerends [PRA 51, 170 (1995)]

$$F[\rho_B] - F[\rho_A] = \int_A^B dt \int d^3r \; v[\rho_t] \frac{d\rho_t(\vec{r})}{dt}$$



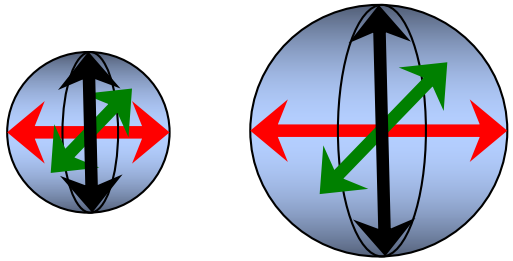
Which path of densities?

In the works by A. Gaiduk *et al.*, **possible choices are discussed** [cf. e.g. J. Chem. Theory Comput. 5, 699 (2009)].

t - scaling

$$\rho_t(\vec{r}) = t^3 \rho(t\vec{r})$$

This looks familiar to nuclear physicists as the **scaling model for the GMR**.



In principle, it can be generalised to other shapes.

We have applied the line-integration formula **for the first time in the nuclear case.**

We have shown that we can indeed reconstruct the EDF.

Simple Skyrme (t_0-t_3) EDF.

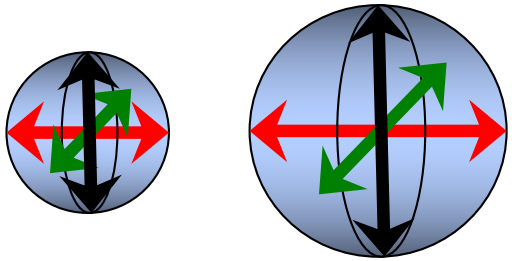
$$\left(-\frac{\hbar^2\nabla_i^2}{2m}+v[\rho]+v_{\rm ext}\right)\phi_i(\vec{r})=\varepsilon_i\phi_i(\vec{r})$$

When we invert the relation between densities and potentials we obtain: $v = v[\rho] + v_{\rm ext}$

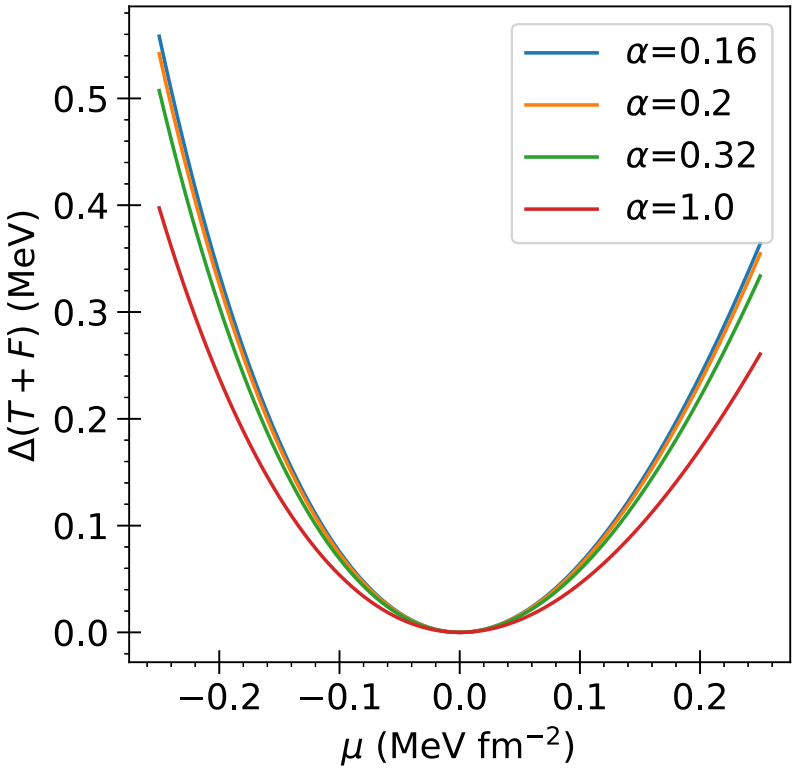
The relevant information is $v[\rho] = \dfrac{\delta F}{\delta \rho}$

We must use a density path in which the external potential is known along with the density

$$v_{\rm ext} = \mu r^2$$



Reconstruction of E[ρ]



What information do we get when we reconstruct the energy?

In the **case at hand**, we have correctly reproduced the EDF.

$$\mathcal{E} = \frac{1}{2}\left(t_0 + \frac{t_3}{6}\rho^\alpha\right)\left(\rho^2(\vec{r}) - \frac{1}{2}\rho_p^2(\vec{r}) - \frac{1}{2}\rho_n^2(\vec{r})\right)$$

We are indeed **sensitive to the exponent α.**

Appropriate strategies must be devised if we start from *ab initio* results.

G. Accorto *et al.*, Phys. Rev. C101, 024315 (2020).

A. Liardi *et al.*, Phys. Rev. C105, 034309 (2022).

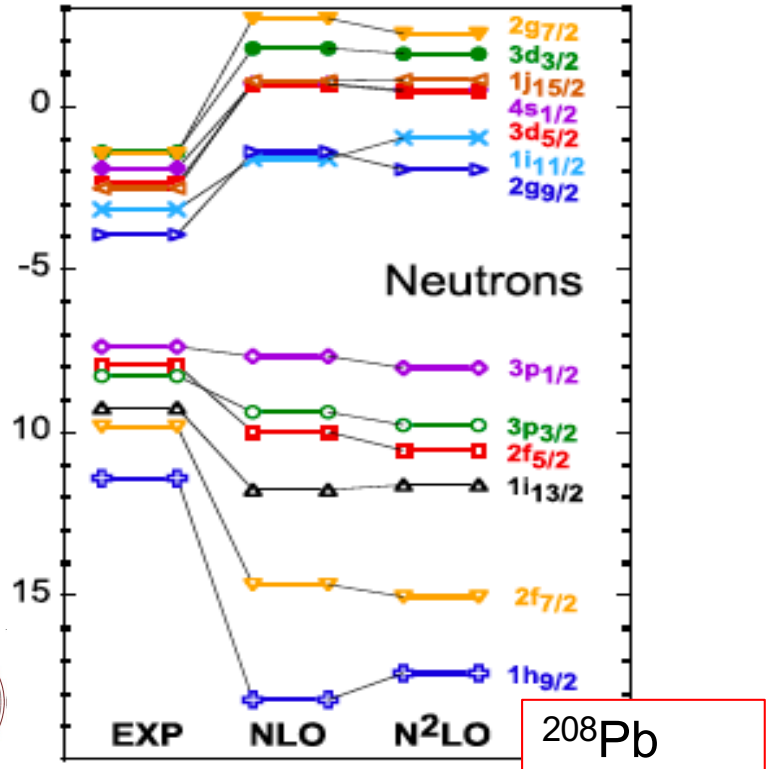
- Many-body correlations (“PVC vs GW”)

Limitations of nuclear DFT

Single-particle states and the associated transfer reaction cross sections or spectroscopic factors (S_n) are not within the DFT framework.

$$S_n \equiv \int d^3r \; |\phi_n(\vec{r})|^2, \qquad \phi_n(\vec{r}) = \langle n, A-1 | a_{\vec{r}} | A \rangle$$

K. Bennaceur *et al.*, J. Phys. G 44 (2017) 045106

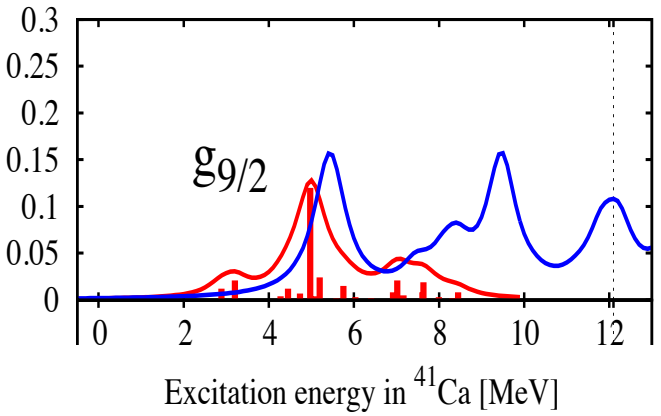


^{208}Pb

Single-particle strength

$9/2^+$ strength in ^{41}Ca (^{40}Ca core)

Red = experiment (d,p)



Our many-body approach

$$H = H_0 + V_{\rm eff}$$

$$\sum_i \varepsilon_i a_i^\dagger a_i + \frac{\delta^2 H}{\delta\rho\delta\rho}$$

κ 

Equations for $G, \Sigma, W, \Pi, \Gamma$ can be derived

- The set of equations for these quantities has been derived in the famous paper(s) by **L. Hedin** for the Coulomb force.
- The validity of this scheme when starting from EDF at 0th order is discussed.

M. Baldo *et al.*, J. Phys. G 42 (2015) 085109

E. Litvinova and P. Schuck,
Phys. Rev. C 100, 064320 (2019)
Phys. Rev. C 102, 034310 (2020)

Hedin's equation

$$G(1,2) = G^0(1,2) + G^0(1,3)\Sigma(3,4)G(4,2)$$

$$\Sigma(1,2) = iG(1,3)\Gamma(3,2,4)W(4,1)$$

$$W(1,2) = \kappa(1,2) + \kappa(1,3)\Pi(3,4)W(4,2)$$

$$\Pi(1,2) = -iG(1,3)G(4,1)\Gamma(3,4,2)$$

$$\Gamma(1,2,3) = \delta(1,2)\delta(1,3) + \frac{\delta\Sigma(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\Gamma(6,7,3)$$

G = Green's function, Σ = self-energy, W = induced interaction, Π = polarization propagator, Γ = vertex function

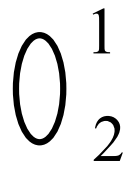
PHYSICAL REVIEW VOLUME 139, NUMBER 3A 2 AUGUST 1965

New Method for Calculating the One-Particle Green's Function with Application to the Electron-Gas Problem*

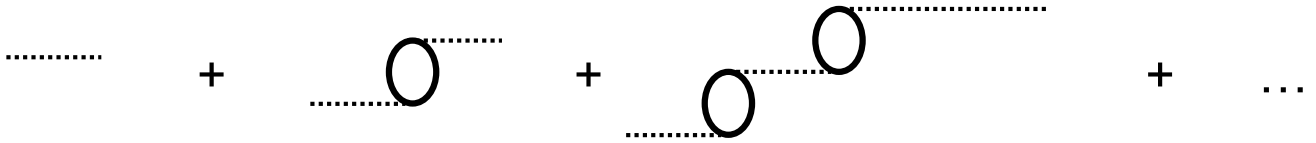
LARS HEDIN†
Argonne National Laboratory, Argonne, Illinois
(Received 8 October 1964; revised manuscript received 2 April 1965)

Vertex function: $\Gamma(1,2,3) \approx \delta(1,2)\delta(1,3)$

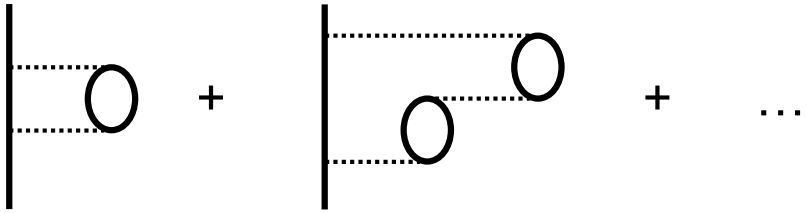
$$\Pi(1,2) = -iG(1,2)G(2,1)$$



$$W(1,2) = \kappa(1,2) + \kappa(1,3)\Pi(3,4)W(4,2)$$



$$\Sigma(1,2) = iG(1,2)W(1,2)$$



$$G(1,2) = G^0(1,2) + G^0(1,3)\Sigma(3,4)G(4,2)$$

We work within this scheme in what follows

$$\Sigma \rightarrow G \rightarrow \Gamma \rightarrow \Pi \rightarrow W$$

Order 0

$$\Sigma = 0$$

$$G = G^0$$

$$\Pi = -iG^0G^0$$

The last is the RPA equation

$$W = \kappa + \kappa\Pi W$$

Order 1

$$\Sigma = iG^0W$$

This is called PVC. Cf. next slide(s)

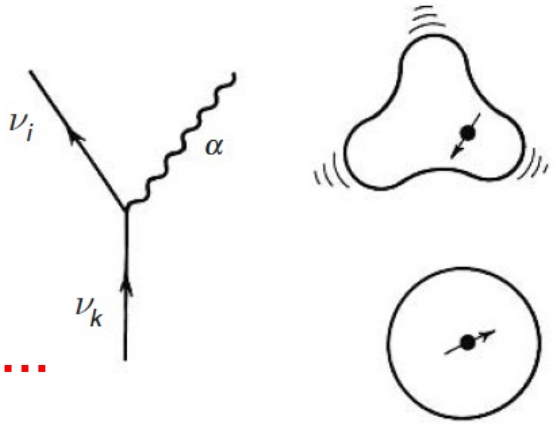
$$G = G^0 + G^0\Sigma G$$

$$\Pi = -iGG$$

$$W = \kappa + \kappa\Pi W$$

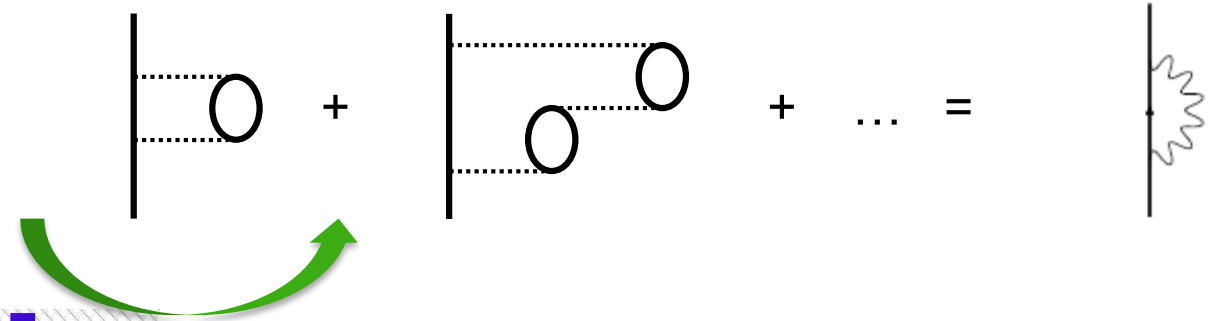
Particle-vibration coupling (PVC)

- The basic idea is that in spherical nuclei there are **single-particle states** and (mainly surface) **collective vibrations.** The spectra result from their **interplay.** (Deformed nuclei: particle-rotation coupling)
- **Vibrations = phonons.**
- Even nuclei: core + 1p-1h + **1p-1h plus phonon …**
- Odd nuclei: core + 1 particle + **1 particle plus phonon …**

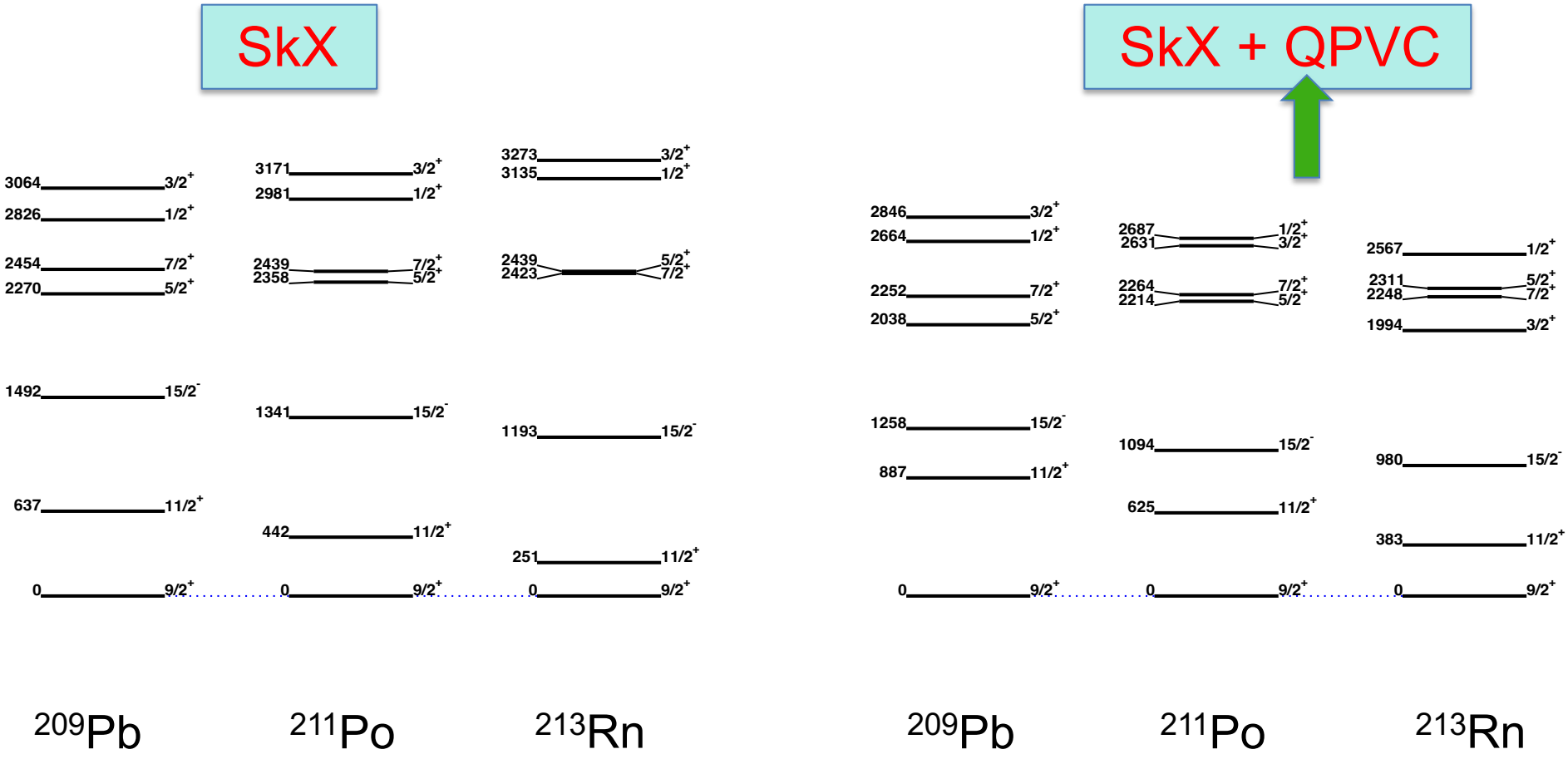


$$\Sigma = iG^0W$$

$$G = G^0 + G^0\Sigma G$$



Shell evolution in exotic nuclei



(Q)RPA+(Q)PVC

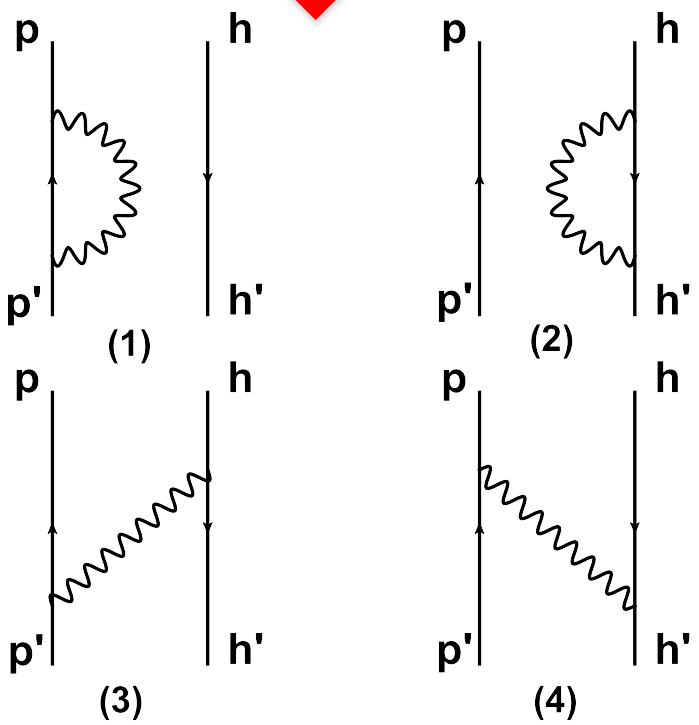
$$\begin{pmatrix} A+\Sigma(E) & B \\ -B & -A-\Sigma^*(-E) \end{pmatrix} \qquad \Sigma_{\mathrm{php'h'}}(E) = \sum_\alpha \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E-E_\alpha+i\eta}$$

The state α is 1p-1h plus one phonon.

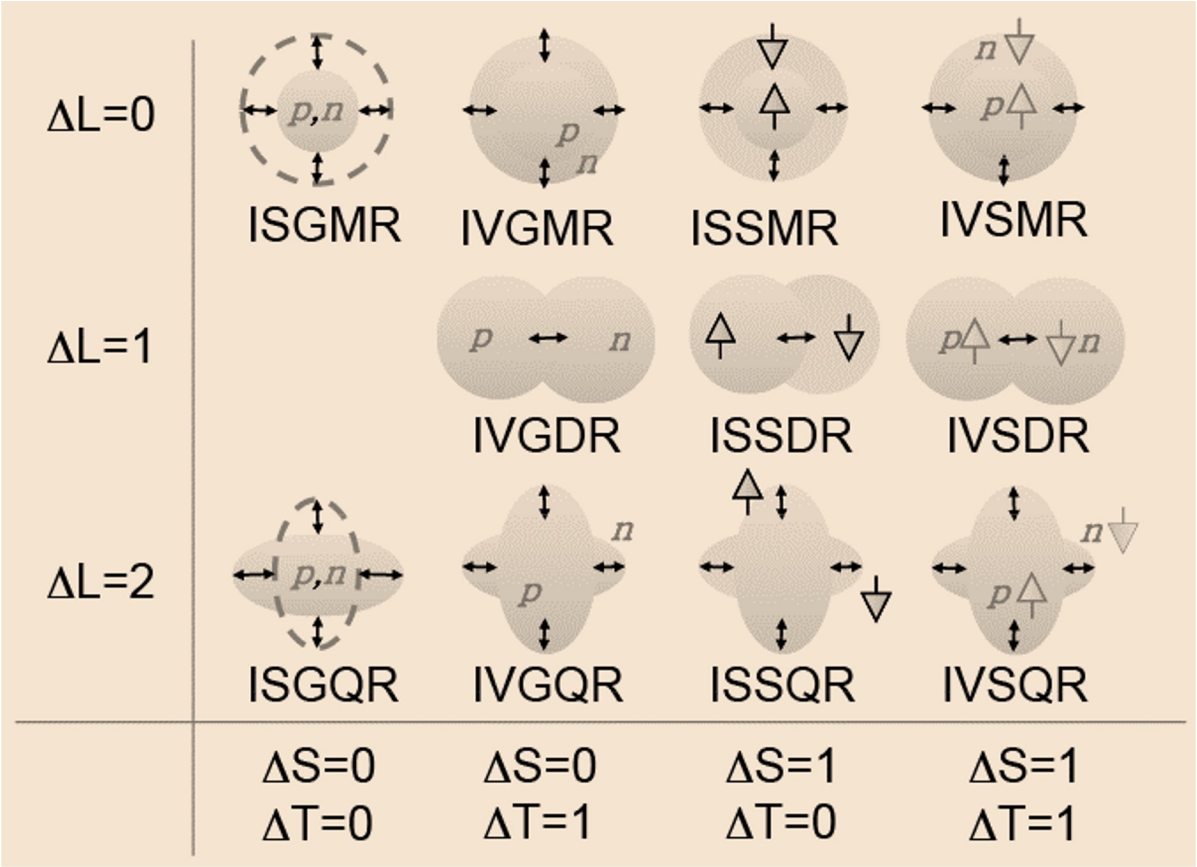
Scheme effective to produce GR widths !

Pauli principle !

$$\Pi = -iGG$$
$$W = \kappa + \kappa\Pi W$$



Giant Resonances

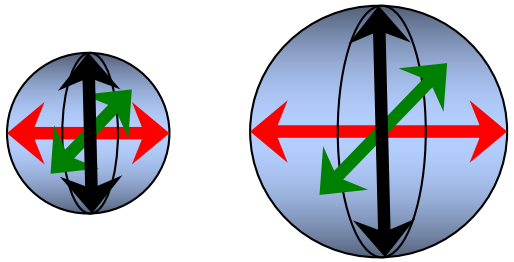


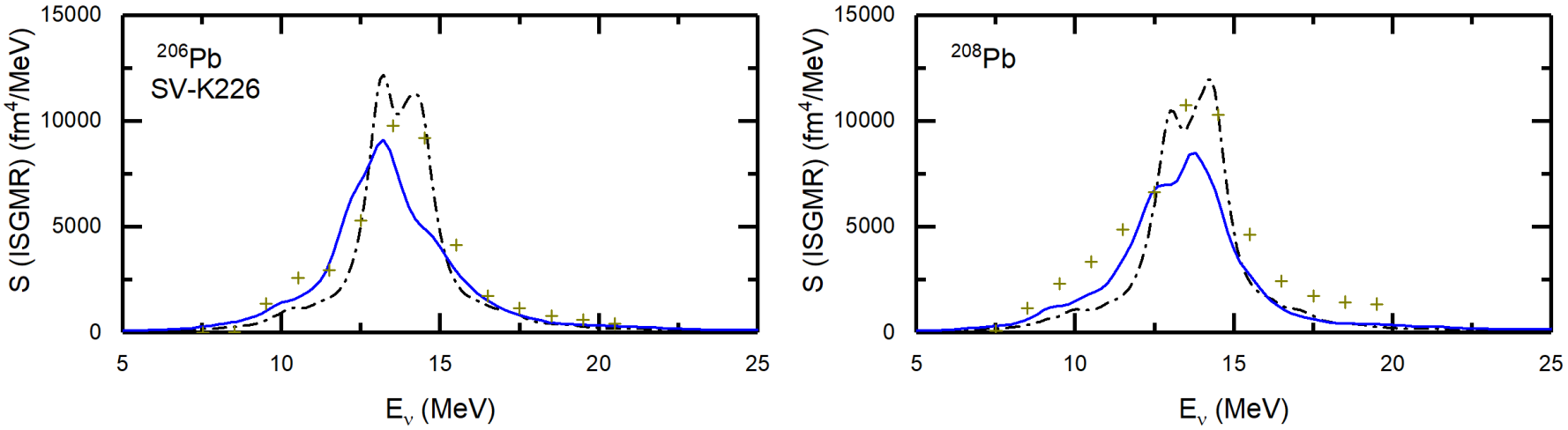
IS = Iso-Scalar
IV = Iso-Vector
S = Spin
G = Giant
M = Monopole
D = Dipole
Q = Quadrupole
O = Octupole

Prominent features of the nuclear response: large peaks in e.g. inelastic spectra.
IVGDR is analogous to a plasmon in a molecular aggregate.

ISGMR in Pb isotopes

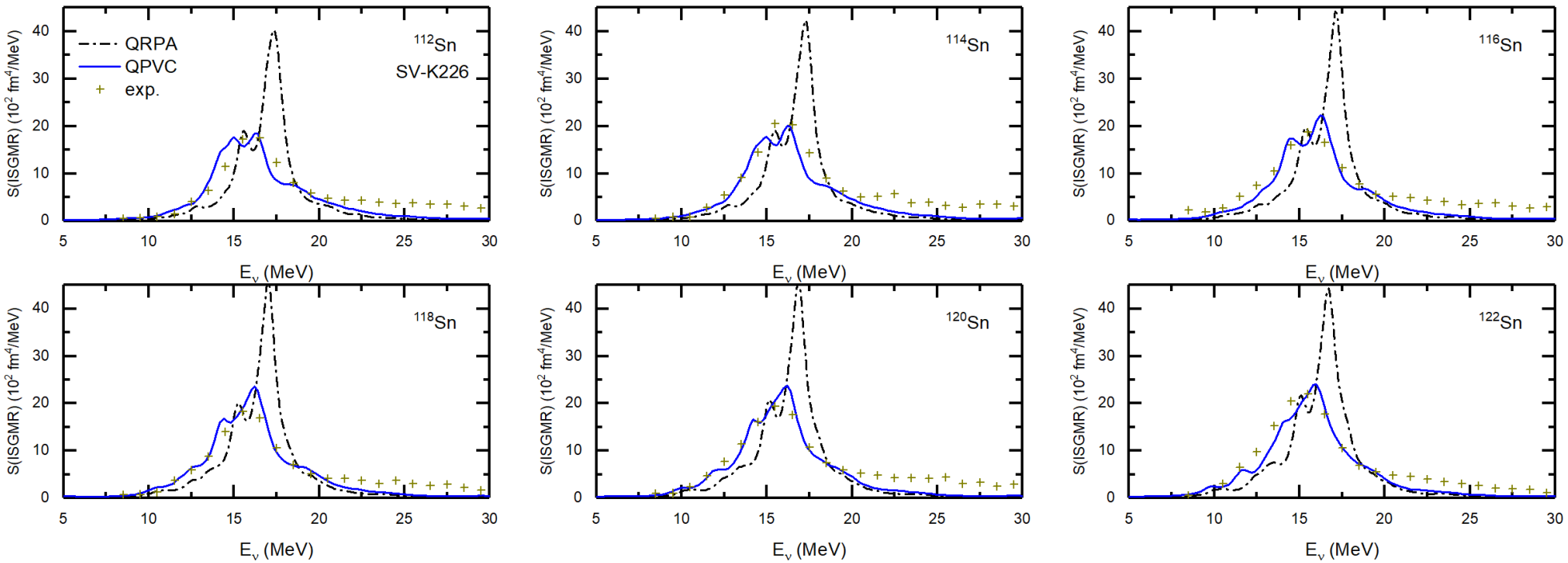
The ISGMR is also called “breathing mode”: its energy should be correlated with the compressibility of nuclear matter.





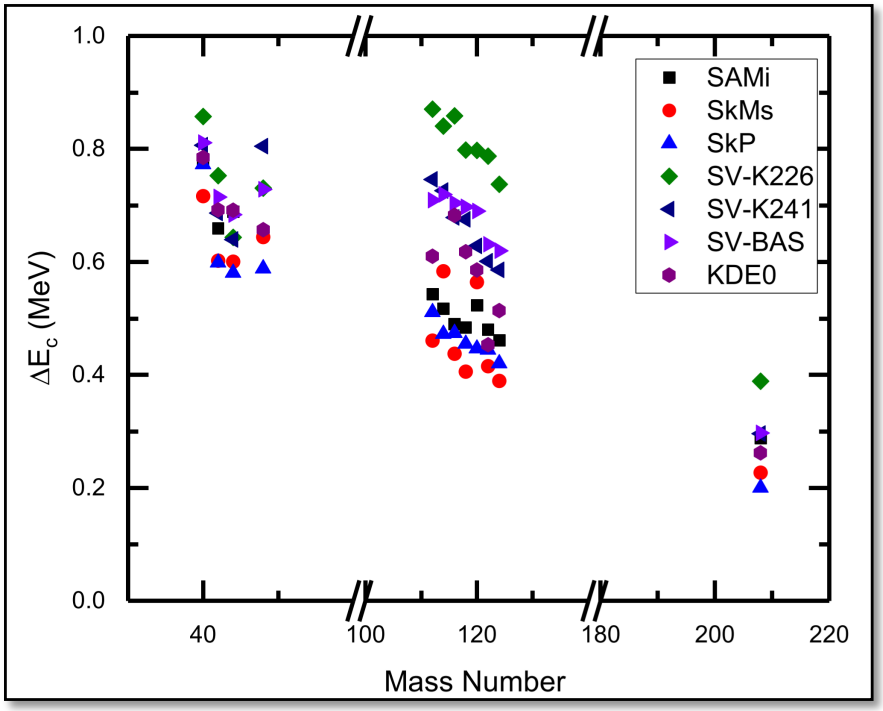
- Exp. data from D. Patel *et al.*, Physics Letters B 735, 387 (2014).

ISGMR in Sn isotopes



- Exp. data from T. Li *et al*., Phys. Rev. Lett. 99, 162503 (2007).
- QPVC reproduces the experimental data quite well.
- The best description is obtained with the Skyrme EDF SV-K226.

The energy shift from QRPA to QPVC

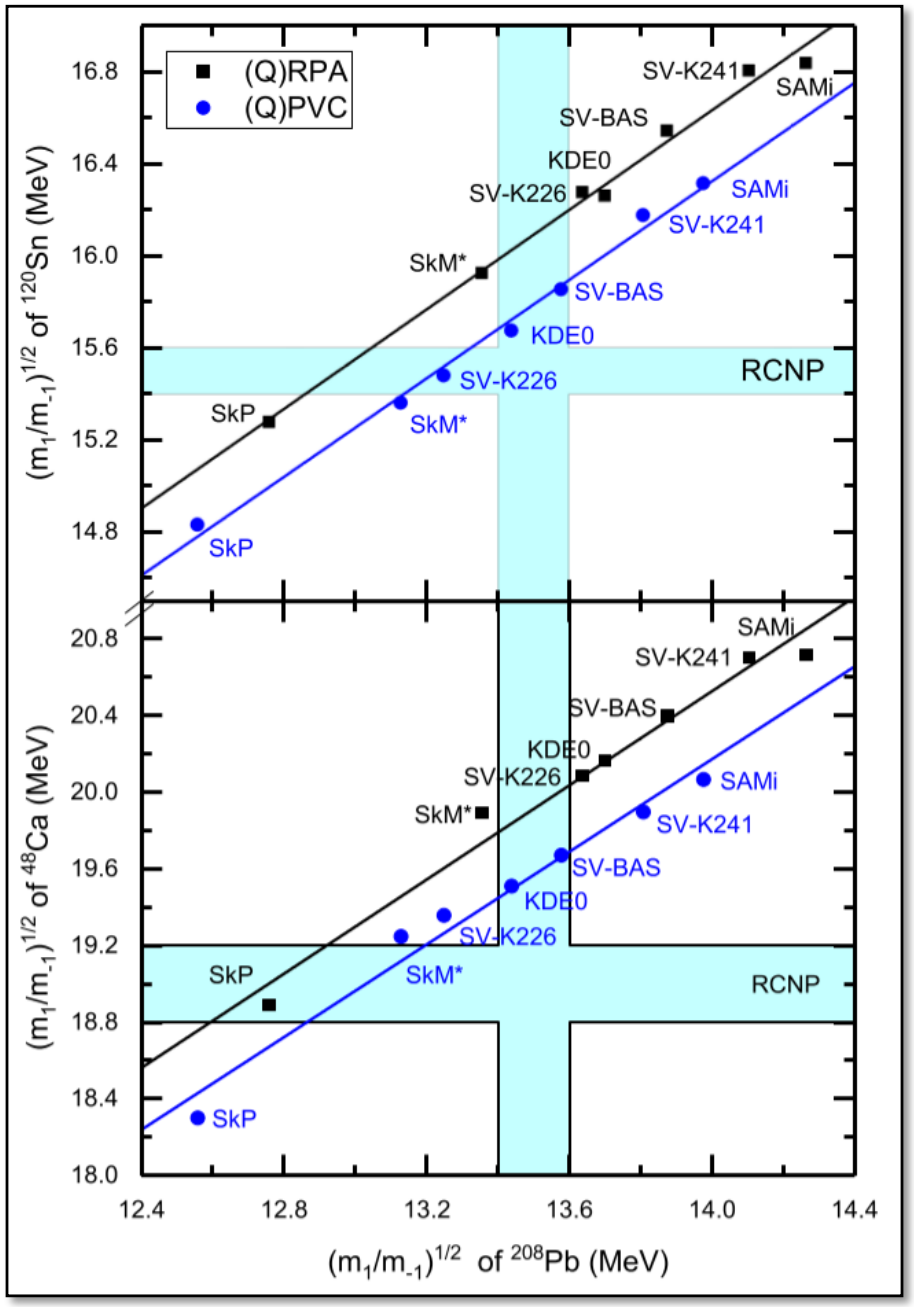


In general, the coupling with the vibrations shifts the mean energies downward.

For monopole, the shift is not large (less than 1 MeV).

There is considerable dispersion among the results from different Skyrme EDFs.

Still, the shift in ^{208}Pb is smaller than for Sn and Ca isotopes.



The ISGMR energy of ^{120}Sn (or ^{48}Ca) and ^{208}Pb can not be described simultaneously at QRPA level

With the inclusion of QPVC effects, a big improvement is achieved.

Within QPVC, the ISGMR energy in ^{208}Pb is consistent with ^{120}Sn.

Z.Z. Li, Y.F. Niu, GC (submitted)

- C. Barbieri, P. Brandolini, F. Marino, X. Roca-Maza, E.Vigezzi (Univ. of Milano and INFN, Italy)
- F. Pederiva (Univ. of Trento and INFN, Italy)
- A. Porro, A. Scalesi (CEA, Saclay, France)
- G. Accorto (Univ. Zagreb, Croatia)
- A. Liardi (Cambridge University, UK)
- A. Lovato (ANL, USA)
- Y.F. Niu, Z.Z. Li (Lanzhou University, China)

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Backup slides

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Nuclear density functional theory

G. Colò

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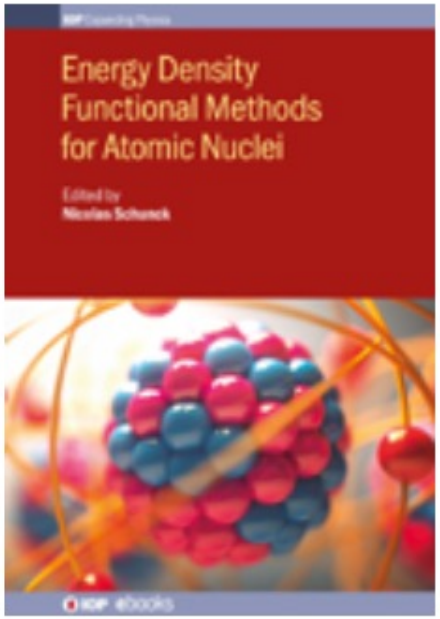

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Nuclei are spin-1/2 fermions and the EDFs can depend on **number or spin densities**.

Generalised densities are obtained by the systematic use of derivative operators.

$$\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$

~~$$\mathbf{s}(\mathbf{r}) = \mathbf{s}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$~~

~~$$\mathbf{j}(\mathbf{r}) = \frac{1}{2i}\left(\nabla - \nabla'\right)\rho(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}}$$~~

$$\tau(\mathbf{r}) = \nabla\cdot\nabla'\rho(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$

$$\mathbf{J}(\mathbf{r}) = \frac{1}{2i}\left(\nabla - \nabla'\right)\otimes\mathbf{s}(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}}$$

~~$$\mathbf{T}(\mathbf{r}) = \nabla\cdot\nabla'\mathbf{s}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$~~

Kinetic energy density

$$T = \int d^3r\ \frac{\hbar^2}{2m}\tau(\mathbf{r})$$

$$\mathbf{J}_{\mu\nu} = \frac{1}{3}\delta_{\mu\nu}J^{(0)} + \frac{1}{2}\sum_{\kappa}\epsilon_{\mu\nu\kappa}J^{(1)}_{\kappa} + J^{(2)}_{\mu\nu}$$

Spin-orbit density

Courtesy: R. Godby

Approaches to the electron-electron interaction

- *Density-functional theory* (for ground-state properties only):

$$\left[-\tfrac{1}{2}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{xc}}(\mathbf{r}) - \varepsilon_i\right]\psi_i(\mathbf{r}) = 0$$

- *Many-body perturbation theory* based on Green's functions:

$$\left[-\tfrac{1}{2}\nabla^2 + V_{\text{ext}} + V_{\text{Hartree}} + \Sigma_{\text{xc}}(\omega) - \omega\right]G(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}')$$

(which, *inter alia*, leads to the quasiparticle equation

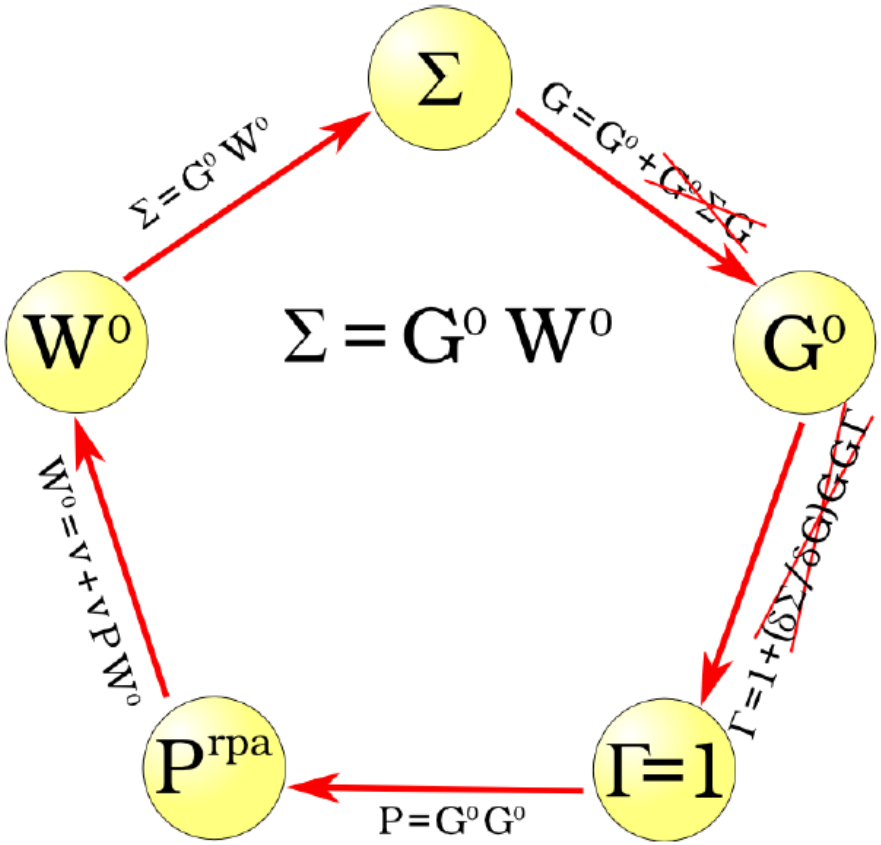
$$\left[-\tfrac{1}{2}\nabla^2 + V_{\text{ext}} + V_{\text{Hartree}} + \Sigma_{\text{xc}}(\varepsilon) - \varepsilon\right]\psi(\mathbf{r}) = 0)$$

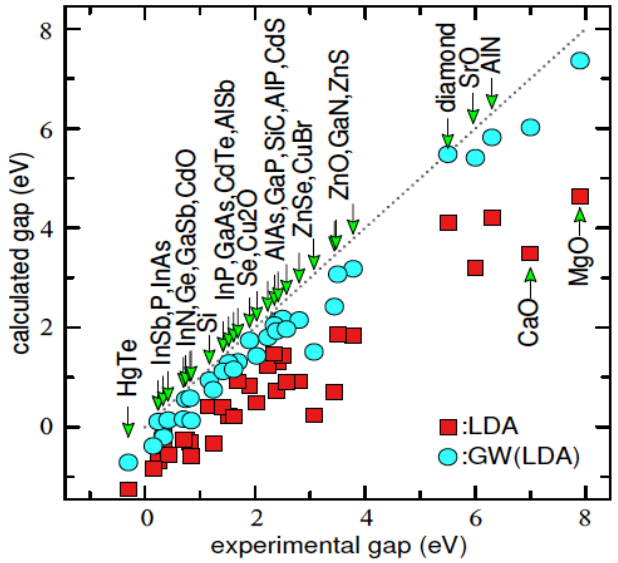
Note the two ways of describing exchange and correlation:

In DFT: $V_{\text{xc}}(\mathbf{r})$ (local, energy-independent potential)

In many-body theory: $\Sigma_{\text{xc}}(\mathbf{r},\mathbf{r}',\omega)$ (non-local, energy-dependent potential)

Hedin's pentagon: possible strategy





van Schilfgaarde *et al.*, PRL **96**, 226402 (2006)