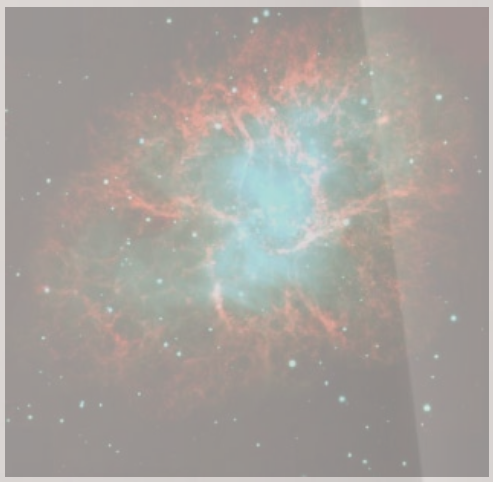
DFT versus many-body Green's function theory for nuclear structure

Gianluca Colò



Università degli Studi and INFN, MIlano

Interdisciplinary symposium on modern DFT - RIKEN, Japan, June 19th-23rd, 2017

Outline

- 1st part: definition of nuclear EDF, and answer to the question "Why can't we get nuclear properties right, if we stay outside DFT ?" (with some examples).

- 2nd part: an implementation of Green's function theory – in almost full analogy with the electronic case (Hedin's scheme).

- Conclusions / Outlook.

Nuclear DFT (I)

$$E = \langle \Psi | \hat{H} | \Psi \rangle \approx \langle \Phi | \hat{H}_{eff} | \Phi \rangle = E[\hat{\rho}]$$

$|\Phi\rangle$ **Slater determinant** $\Leftrightarrow$ $\hat{\rho}$ **1-body density matrix**

Working with exact Hamiltonian and wave function: too hard !

Strategies:

1. Start from a two-body (three-body) effective force and define H = T + V_{eff} [ϱ]. Write the expectation value on a general Slater determinant.
2. Write directly the Energy Density Functional (EDF).

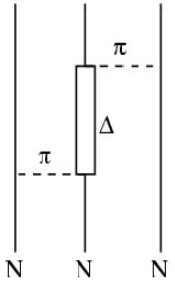
IF THE PARAMETERS ARE FITTED ON EXPERIMENTAL DATA THEY INCLUDE CORRELATIONS.

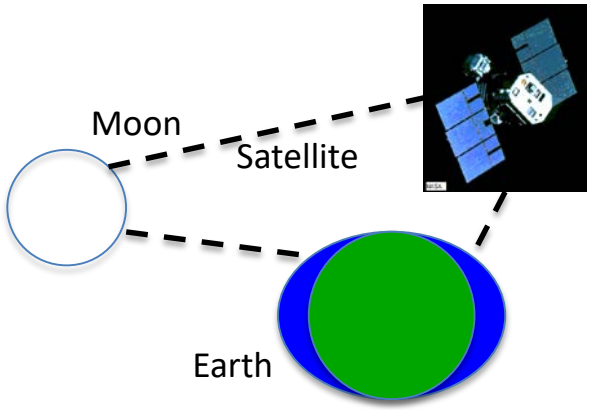
Why not to mimic the Coulomb case ?

- **The interaction in the medium is very strongly renormalized with respect to the force between two nucleons in the vacuum (bare force).**

- **Three-body forces** are mandatory (if not more).

- Green's function theory for three-body forces only recently developed.
A. Carbone *et al.*, Phys. Rev. C 88, 054326 (2013)





- If one starts from bare forces with strong repulsion at short-distance, **Hartree energy/potential is hard to obtain.**

- After all, also bare forces are fitted to data and not unique.

- **For these and other reasons, many prefer to FIT a V_{eff} or an EDF.**

Applicability of DFT

... consistent microscopic framework for a unified description of bulk properties, excitations and reactions!

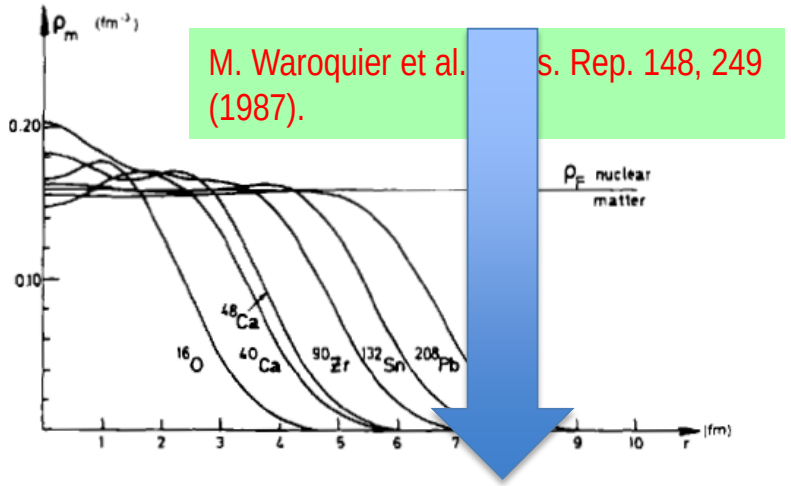
Ab initio:
Quantum Monte Carlo,
No-core Shell Model,
Coupled-Cluster, ...

Density Functionals
(self-consistent mean fields)

Configuration interaction
(Interacting Shell-Model)

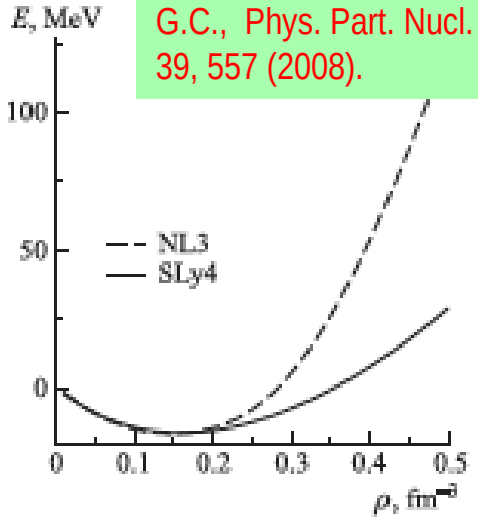
Fitting a V_{eff} or an EDF

- The **empirical saturation point** is always fitted when building an EDF.



M. Waroquier et al. s. Rep. 148, 249 (1987).

$$E = a_V - a_S A^{-1/3} - a_A \frac{(N-Z)^2}{A}$$



G.C., Phys. Part. Nucl. 39, 557 (2008).

E/A OF SYMMETRIC MATTER HAS A MINIMUM AT ϱ_0 = 0.16 fm^{-3}; VALUE AT THE MINIMUM -16 MeV

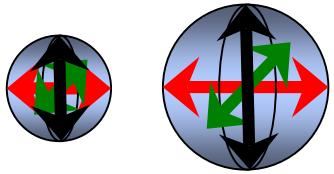
- Then, a number of **MASSES** and **CHARGE RADII** are fitted.

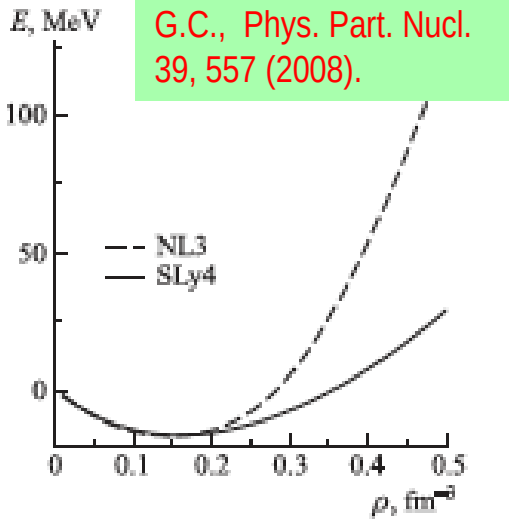
Symmetric and asymmetric nuclear matter

- E/A is called nuclear Equation of State (EoS).

- For symmetric matter we do have information about the **incompressibility**: $K_\infty = 220 \pm 20$ MeV

$$K_\infty = 9\rho_0^2 \frac{d^2}{d\rho^2}\frac{E}{A}\bigg|_{\rho_0}$$





G.C., Phys. Part. Nucl. 39, 557 (2008).

- There is some information about asymmetric matter, yet much less. **S is the symmetry energy.**

$$\beta \equiv \frac{\rho_n - \rho_p}{\rho} \qquad \frac{E}{A}(\rho,\beta) = \frac{E}{A}(\rho,\beta=0) + S(\rho)\beta^2$$

- Current knowledge: $S(\rho_0) = 32 \pm 3$ MeV $\qquad L \equiv 3\rho_0 S'(\rho_0) = 59 \pm 32$ MeV

(Pure) neutron matter (β=1)

$$\frac{E}{A}(\rho,\beta) = \frac{E}{A}(\rho,\beta=0) + S(\rho)\beta^2$$

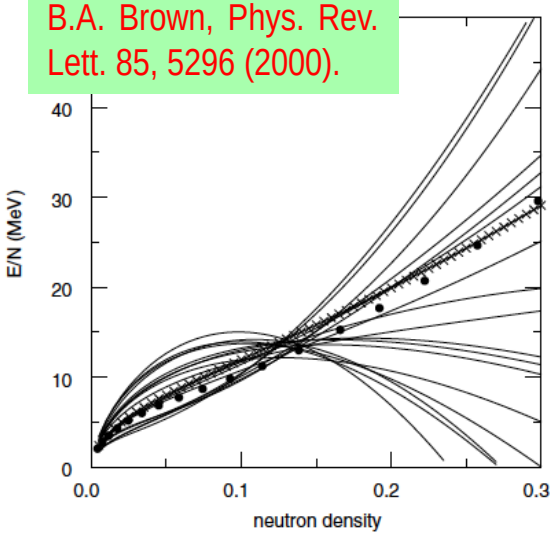
- Within the "quadratic" approximation, S is the difference between the energy per particle in neutron matter and symmetric matter:

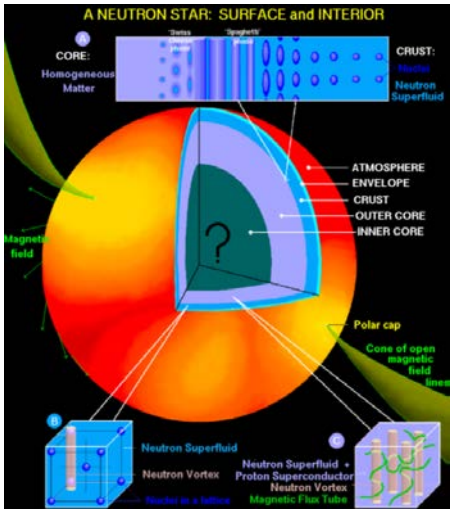
$$S \equiv \frac{E}{A}(\beta=1) - \frac{E}{A}(\beta=0)$$

- We have incomplete knowledge of neutron matter, and it may desirable to obtain it from e.g. more fundamental calculations.

- This is not a "toy system". Neutron stars exist !

B.A. Brown, Phys. Rev. Lett. 85, 5296 (2000).





Nuclear saturation with constant V: no way !

- At saturation density: $k_F \approx 1.33\ \mathrm{fm}^{-1}$ $T_F \approx 40\ \mathrm{MeV}$
- A two-body potential with constant matrix elements would give at the Fermi energy

$$E/A \approx T_F + V \approx -16\ \mathrm{MeV}$$

- The same potential would give in a mean-field framework

$$E = \sum_i \left(T_i + \frac{V}{2} \right) = A \left(\frac{3}{5} T_F + \frac{V}{2} \right)$$

- The two equations are incompatible !

T. Nakatsukasa *et al.*, Rev. Mod. Phys. 88, 045004 (2016)

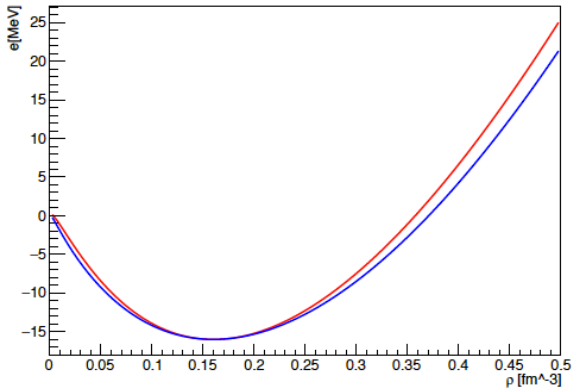
Finite-range is not enough: need of more ranges, or exchange forces

- Due to its short-range, the Fourier transform of the nucleon-nucleon force does not have a strong **k**-dependence
- **One must add explicit velocity dependence or exchange terms**
- Gaussian or Yukawa interactions with exchange terms reproduce saturation:

$$V = S\left[(1-m) + mP_M\right] e^{-|\vec{r}_1 - \vec{r}_2|/\mu^2}$$

- Increasing the number of ranges give more and more flexibility to fit K_∞, $S(\varrho_0)$, L …
- (Very) wrong effective mass !

$$m^*/m \approx 0.2 - 0.3$$



G. Accorto, R. Romano, A. Rancati, X. Roca-Maza, G.C. (to be published).

Reminder on effective mass

$$E = \frac{\hbar^2 k^2}{2m} + \Sigma(k, E)$$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} + \frac{d\Sigma}{dE}\frac{dE}{dk} + \frac{d\Sigma}{dk}$$

$$\frac{dE}{dk}\left(1 - \frac{d\Sigma}{dE}\right) = \frac{\hbar^2 k}{m} + \frac{d\Sigma}{dk}$$

If we wish to define

$$E \equiv \frac{\hbar^2 k^2}{2m^*} \rightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m^*}$$

then

$$\frac{\hbar^2 k}{m^*} = \left(1 - \frac{d\Sigma}{dE}\right)^{-1}\left(\frac{\hbar^2 k}{m} + \frac{d\Sigma}{dk}\right)$$

$$\frac{m}{m^*} = \left(1 - \frac{d\Sigma}{dE}\right)^{-1}\left(1 + \frac{m}{\hbar^2 k}\frac{d\Sigma}{dk}\right)$$

Here, E is the single-particle energy, NOT the total energy.

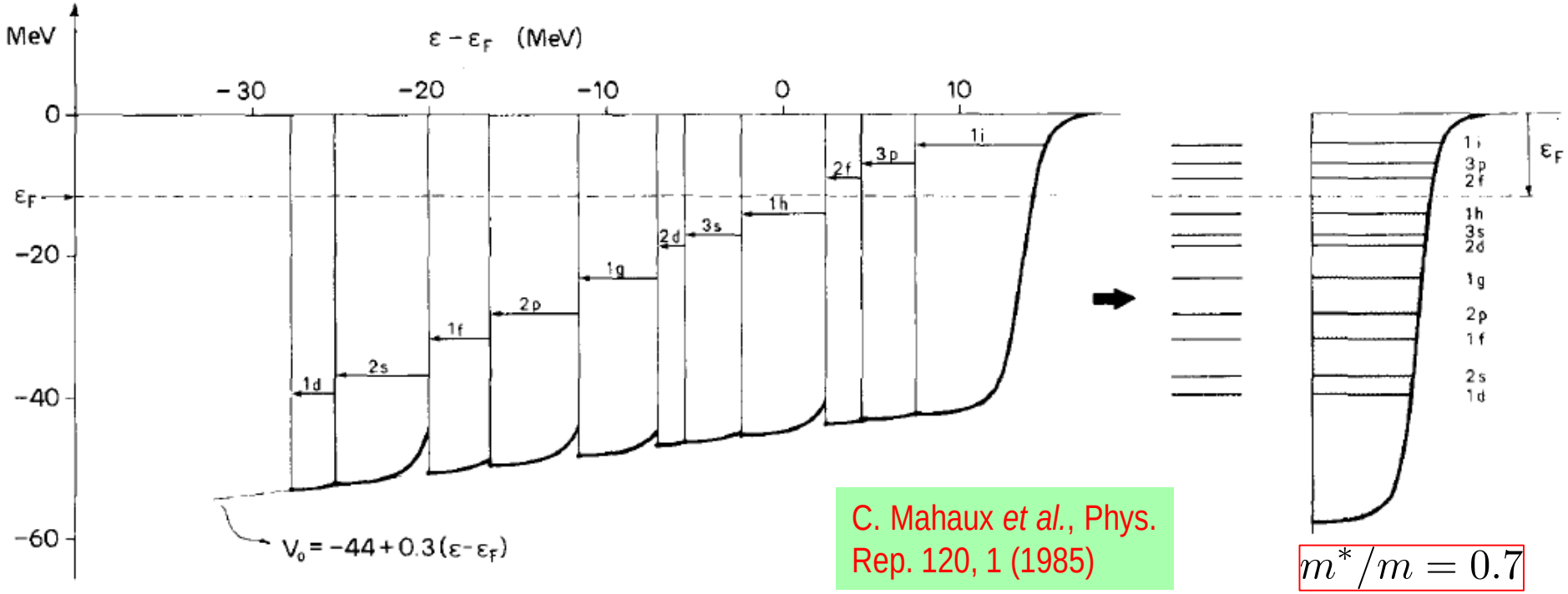
The effective mass, in particular m*/m, is related to the density of s.p. states.

$$m^*/m \approx 0.7 - 1$$

First term: E-mass

Second term: k-mass

Effective mass vs. levels in finite nuclei



C. Mahaux *et al.*, Phys. Rep. 120, 1 (1985)

$m^*/m = 0.7$

Experimental main peaks of transfer reactions like (d,p) can be reproduced by different Woods-Saxon potentials. Sometimes this is equivalent to a single potential if m is introduced.*

The empirical value of m*/m is between 0.7 and 1.

Nuclear DFT (II)

The only way to reconcile **to some extent** different properties of nuclei are **density-dependent interactions. Ultimately, these are just "*EDF generators*" !**

$$E = \int \mathcal{E}[\rho] \; d^3r$$

- Mechanism for saturation
- Flexibility (i.e., enough terms) to account for the many features of finite nuclei and of the EoS
- Suitable for extensive computational efforts
- Linkable to more fundamental theories (?)

The Gogny force

$$\hat{v}_{\text{Gogny}}(r_{12}) = \sum_{j=1}^{2} \mathrm{e}^{-(r_{12}/\mu_j)^2}\left(W_j + B_j \hat{P}_\sigma - H_j \hat{P}_\tau - M_j \hat{P}_\sigma \hat{P}_\tau\right)$$

$$+ t_3\left(1 + x_0 \hat{P}_\sigma\right)\delta(r_{12})\rho^\alpha\left(\frac{r_1 + r_2}{2}\right) + \mathrm{i}W_{ls}(\hat{\sigma}_1 + \hat{\sigma}_2)\cdot \hat{k}^\dagger \times \delta(r_{12})\hat{k}$$

$P_\tau = \frac{1+\vec{\tau}_1\cdot\vec{\tau}_2}{2}$

13 free parameters.

- There are two Gaussians with different ranges and spin/isospin dependence
- The introduction of a density-dependent term seemed unavoidable. This must be zero-range.
- The last term (spin-orbit) is zero-range for simplicity.
- The great advantage of the Gogny force is that it seems adequate not only to enter the HF equations but to describe also *nuclear superfluidity.*

The Skyrme force

attraction

$$\hat{v}_{\rm Sk}(\boldsymbol{r}_{12}) = t_0(1+x_0\hat{P}_\sigma)\delta(\boldsymbol{r}_{12}) + \frac{1}{2}t_1(1+x_1\hat{P}_\sigma)(\hat{\boldsymbol{k}}^{\dagger 2}\delta(\boldsymbol{r}_{12}) + \delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}^2)$$
$$+ t_2(1+x_2\hat{P}_\sigma)\hat{\boldsymbol{k}}^\dagger \cdot \delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}} + \frac{1}{6}t_3(1+x_3\hat{P}_\sigma)\delta(\boldsymbol{r}_{12})\rho^\alpha\left(\frac{\boldsymbol{r}_1+\boldsymbol{r}_2}{2}\right)$$
$$+ \mathrm{i}W_0(\hat{\sigma}_1+\hat{\sigma}_2)\cdot\hat{\boldsymbol{k}}^\dagger \times \delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}.$$

short-range repulsion

$$k = \frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$

- There are velocity-dependent terms which mimick the finite-range. They are related to m*.
- The last term is a zero-range spin-orbit.
- In total: 10 free parameters to be fitted (typically).

Let us see how it works in practice in a simplified case. **A simple two-body force generates E ~ ρ^2.** NOTE: In this slide we call E *only* the potential energy part.

$$t_0\delta(r_{12}) + \frac{1}{6}t_3\delta(r_{12})\rho^\alpha$$

$$E = \frac{1}{2}\sum_{ij}\langle ij|V(1-P_{12})|ij\rangle = \frac{1}{2}\sum_{ij}\int d^3r_1 d^3r_2\ \psi_i^*(r_1)\psi_j^*(r_2)f[\rho(r)]\delta(r_{12})(1-P_\sigma P_\tau)\psi_i(r_1)\psi_j(r_2)$$

$$P_\sigma = \frac{1+\sigma_1\sigma_2}{2},\ \text{and}\ P_\tau = \delta(q_i,q_j)$$

$$E = \frac{1}{2}\sum_{ij}\int d^3r\ \psi_i^*(r)\psi_j^*(r)f[\rho(r)](1-\frac{1}{2}\delta(q_i,q_j))\psi_i(r)\psi_j(r)$$

$$E = \frac{1}{2}\int d^3r\ (t_0 + \frac{t_3}{6}\rho^\alpha)(\rho^2(r) - \frac{1}{2}\rho_p^2(r) - \frac{1}{2}\rho_n^2(r))$$

This is the potential energy. The KS equation reads

$$[-\frac{\hbar^2}{2m}\nabla^2 + U]\psi_i = \epsilon_i\psi_i$$

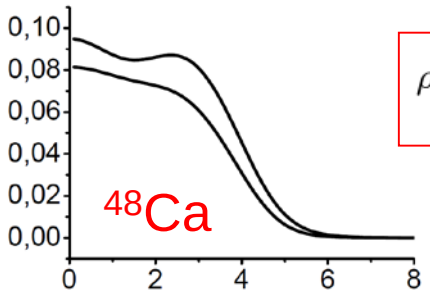
$$\frac{\delta E}{\delta\rho} \equiv U = t_0(\rho - \frac{1}{2}\rho_q) + \frac{1}{12}t_3[(\alpha+2)\rho^{\alpha+1} - \rho^\alpha\rho_q - \frac{1}{2}\alpha\rho^{\alpha-1}(\rho_p^2+\rho_n^2)]$$

More general EDFs (I)

- A strategy may be to consider **all possible densities** (including spin densities, isospin densities, gradients …).

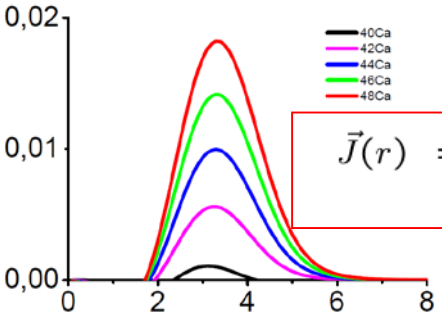
$$\vec{\nabla}\rho$$

$$\tau = \sum_i |\vec{\nabla}\phi_i|^2$$



$$\rho(r) = \sum_{i\in \mathrm{OCC}} \frac{(2j_i+1)}{4\pi r^2} u_i^2(r)$$

$$\vec{J} = \sum_{i,\sigma,\sigma'} \phi_i^\dagger \vec{\nabla}\phi_i \times \langle\sigma'|\vec{\sigma}|\sigma\rangle$$



$$\vec{J}(r) = \sum_{i\in \mathrm{OCC}} 2\,(2j_i+1)\,\langle\,\vec{\ell}\cdot\vec{s}\,\rangle \frac{\vec{r}}{r^4} u_i^2(r)$$

- **Non-locality** well mocked up by gradients, kinetic energy density etc. - **although there are non-local functionals, there does not seem to be strong need**.

Analogies with electronic DFT

FIGURE 1. Jacob's ladder of density functional approximations. Any resemblance to the Tower of Babel is purely coincidental. Also shown are angels in the spherical approximation, ascending and descending. Users are free to choose the rungs appropriate to their accuracy requirements and computational resources. However, at present their safety can be guaranteed only on the two lowest rungs.

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

$$\mathcal{E} = \frac{\hbar}{2m}\tau + \frac{1}{4}t_0[(2+x_0)\rho^2 - (2x_0+1)(\rho_p^2+\rho_n^2)]$$

$$+\frac{1}{24}t_3\rho^\alpha[(2+x_3)\rho^2 - (2x_3+1)(\rho_p^2+\rho_n^2)]$$

$$E_{\rm xc}^{\rm mGGA} = \int d^3r\ f(\rho,\nabla\rho,\nabla^2\rho,\tau)$$

$$+\frac{1}{8}[t_2(2+x_1)+t_2(2+x_2)]\rho\tau$$

$$E_{\rm xc}^{\rm GGA} = \int d^3r\ f(\rho,\nabla\rho)$$

$$+\frac{1}{8}[t_2(2x_2+1)-t_1(2x_1+1)](\tau_p\rho_p+\tau_n\rho_n)$$

$$E_{\rm xc}^{\rm LDA\ or\ LSDA} = \int d^3r\ \rho(r)e_{\rm xc}^{\rm unif}[\rho]$$

$$+\frac{1}{32}[3t_1(2+x_1)-t_2(2+x_2)](\vec{\nabla}\rho)^2$$

$$-\frac{1}{32}[3t_1(2x_1+1)+t_2(2x_2+1)][(\vec{\nabla}\rho_p)^2+(\vec{\nabla}\rho_n)^2]$$

$$+\frac{1}{2}W_0[\vec{J}\cdot\vec{\nabla}\rho+\vec{J}_p\cdot\vec{\nabla}\rho_p+\vec{J}_n\cdot\vec{\nabla}\rho_n]$$

$$-\frac{1}{16}(t_1x_1+t_2x_2)J^2+\frac{1}{16}(t_1-t_2)(J_p^2+J_n^2)$$

More general EDFs (II)

- Question: at which order should one **stop the gradient expansion** ? The answer is likely to be related to the high momentum cutoff of the theory (EFT philosophy).

$$k = \frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$

- All possible terms for EDFs (those compatible with symmetries) are **too many**.

PHYSICAL REVIEW C **78**, 044326 (2008)

Local nuclear energy density functional at next-to-next-to-next-to-leading order

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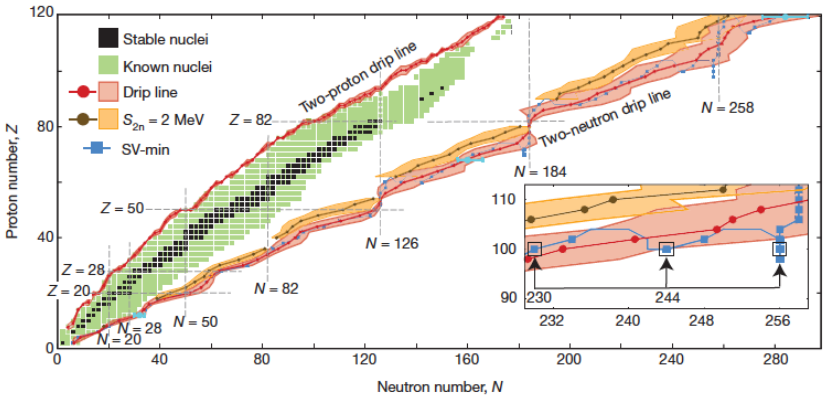
(Received 31 July 2008; published 27 October 2008)

We construct nuclear energy density functionals in terms of derivatives of densities up to sixth, next-to-next-to-next-to-leading order (N^3LO). A phenomenological functional built in this way conforms to the ideas of the density matrix expansion and is rooted in the expansions characteristic to effective theories. It builds on the standard functionals related to the contact and Skyrme forces, which constitute the zero-order (LO) and second-order (NLO) expansions, respectively. At N^3LO, the full functional with density-independent coupling constants, and with the isospin degree of freedom taken into account, contains 376 terms, whereas the functionals restricted by Galilean and gauge symmetries contain 100 and 42 terms, respectively. For functionals additionally restricted by the spherical, space-inversion, and time-reversal symmetries, the corresponding numbers of terms are equal to 100, 60, and 22, respectively.

Masses and drip lines

- Typical energy density functionals have errors ≈ MeV for the masses. It means about 0.1 % to 1 % (!).
- However, we are often interested in differences of masses, for instance for nuclear reactions or nuclear decays.
- GGA or mGGA had few % on such differences.
- The Bruxelles-Montréal collaboration designed specific Skyrme forces for mass systematics. Quite successful at the expense of *ad hoc* terms.

J. Erler *et al.*, Nature 486, 509 (2012) - SEDF



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Masses and radii of neutron stars

Classical gravity (Newton)

$$\frac{dP(r)}{dr} = -\frac{Gm(r)\varepsilon(r)}{r^2c^2}$$

General relativity corrections (TOV)

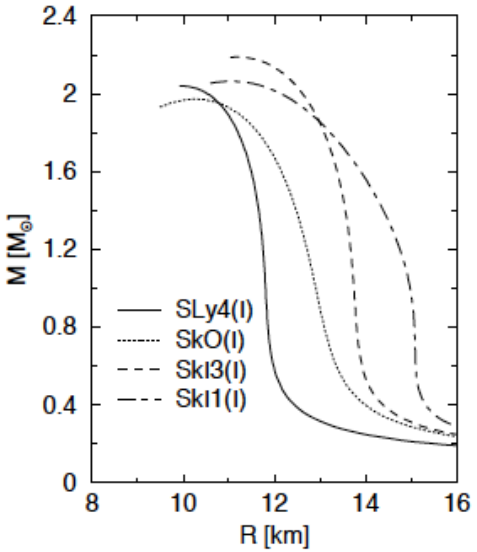
$$\frac{dP(r)}{dr} = -\frac{Gm(r)\varepsilon(r)}{r^2c^2}\frac{\left(1+\frac{P(r)}{\varepsilon(r)}\right)\left(1+\frac{4\pi r^3 P(r)}{\varepsilon(r)}\right)}{1-\frac{2Gm(r)}{rc^2}}$$

One has to input P(ϱ) from the nuclear EOS.

Benchmark ?

Warnings !

J. Stone *et al.*, Phys. Rev. C 68, 034324 (2003).



Too many functionals ?

Eighty-seven parametrizations of the Skyrme interaction, published since 1972 [35], were selected for the analysis presented in this paper. In the order of publication date, these are as follows: SI and SII [22], SkT [36], SIII, SIV, SV, SVI [37], SVII, SIII* [38], SkM [18], SGI, SGII [39], SkM* [40], RATP [41], SkT1-SkT9 [42], SkP [43], E, Es, Z, Zs, Zs*, Rs, Gs [44], SkMP [45], SkSC1-SkSC3 [46], SkSC4 [47], SkSC5, SkSC6, SkSC10 [21], SkI1-SkI5 [48], SLy1-SLy10 [49], SkM1 [50], Skyrme1′ [17], SkI6 [51], SLy230a [23], SKXce, SKXm, SKX [52], SkO, SkO′ [53], MSk1-MSk6 [54], SKRA [55], MSk7 [56], MSk5*, v110-v070 [57], BSk1 [58] and Skz-1, Skz0-4 [59]. The list is not fully

Many-body theory vs. DFT

Theory ensures that an exact Energy Density Functional (EDF) exists.

$$E = E\left[\rho_q \text{ plus gradients, spin densities, } \ldots\right]$$

No exact prescription on how to build it !

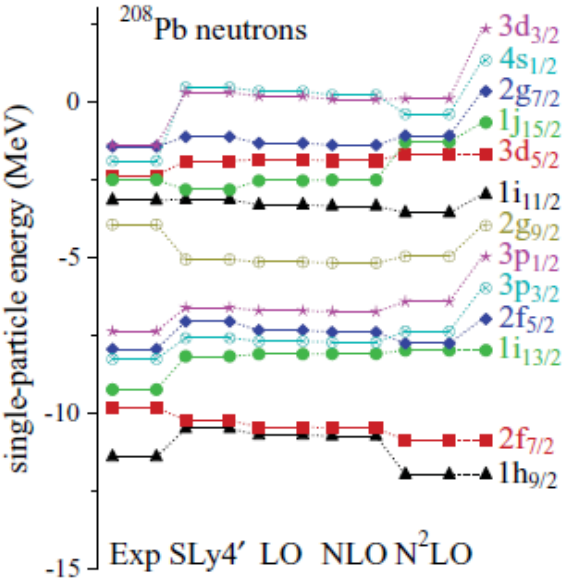
First motivation of our study: if the practical realization of the EDF has shortcomings, other kinds of calculations are useful.

Second motivation of our study: Some phenomena are, by definition, outside the EDF framework: **single-particle states, fragmentation of the s.p. and collective strength** …

Single-particle shell structure

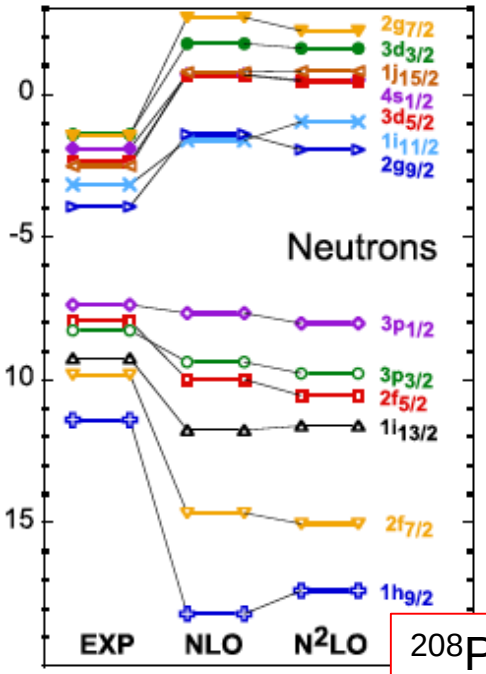
Single-particle states and the associated spectroscopic factors (S_n) are hard to get in the DFT framework. Yet, there is large systematics and even information about the evolution far from stability.

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



Left:
M. Stoitsov *et al.*, Phys. Rev. C 82, 054307 (2010).

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



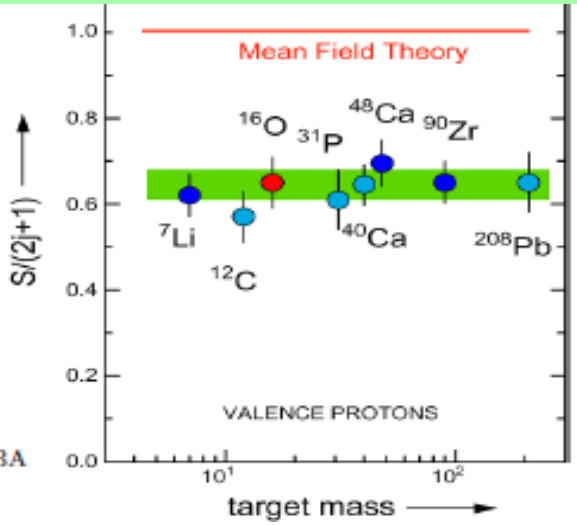
208Pb

Spectroscopic factors

M.B. Tsang *et al.*, Phys. Rev. Lett. 95, 222501 (2013)

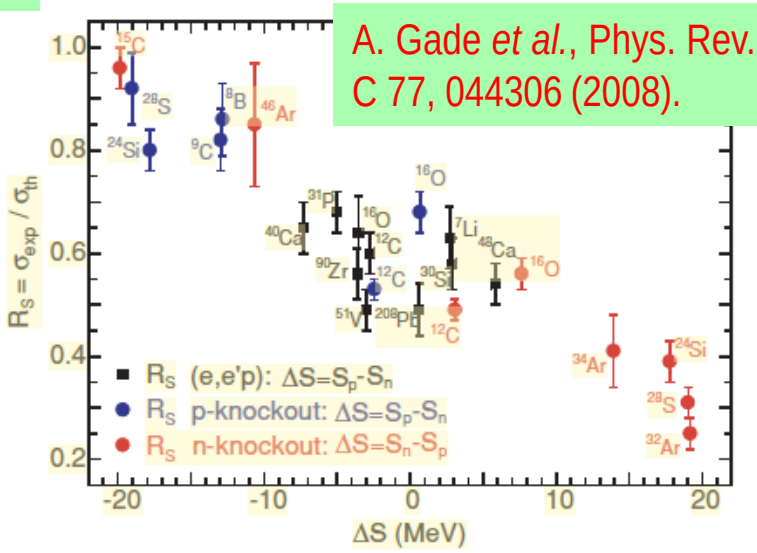
- Not true observables (at best, defined within $\pm$ 20-30%).
- Nevertheless, we can qualitatively say that in stable nuclei states around the Fermi surface are “quasi-particle” states (occupancies around 60-70%) while such approximation tends to break for deeper states.
- Cf. also the plot as a function of the neutron excess.

L. Lapiskas, Nucl. Phys. A 553, 297c (1993).



$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{exp}} = S^2 \left(\frac{d\sigma}{d\Omega}\right)_{\text{DWBA}}$$

A. Gade *et al.*, Phys. Rev. C 77, 044306 (2008).

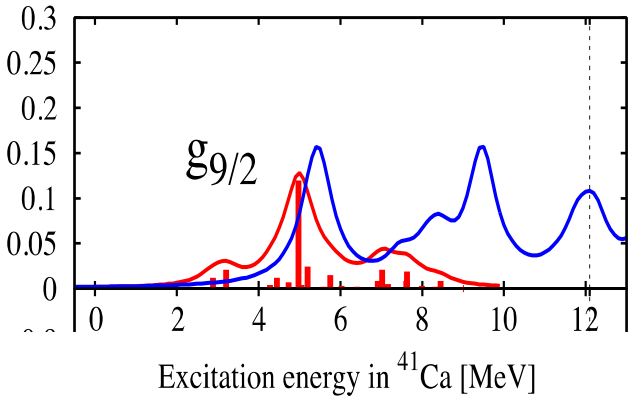


Strength fragmentation

We would like to have a model that explains **fragmentation and widths of single-particle and collective strength** in a consistent fashion.

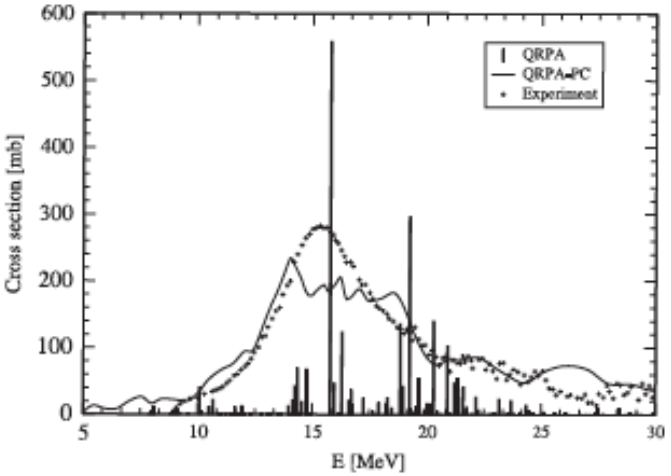
Single-particle strength

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



Collective strength

Photoabsorbtion (dipole) cross section in ^{120}Sn



Our many-body approach

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

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

κ 

Equations for G, M, W, Π, Γ can be derived

- Our equations are formally the same as those by L. Hedin for the Coulomb force.
- We claim that **the so-called particle vibration coupling approach of nuclear structure can be recast as a well-defined approximation scheme** within this framework.
- Start from the basis of the eigenstates of H[ϱ] (?)

Hedin's equations

$$1 \equiv (\vec{r}_1, t_1)$$

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

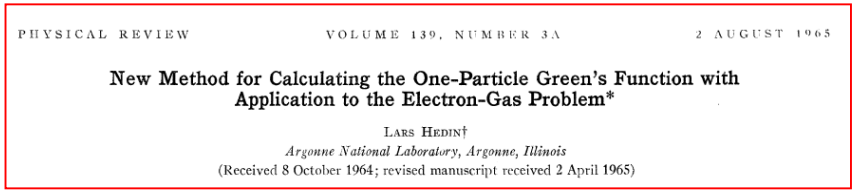
$$M(1,2) = iG(1,3)\Gamma(3,2,4)W(4,1)$$

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

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

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

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



PHYSICAL REVIEW VOLUME 139, NUMBER 3A 2 AUGUST 1965

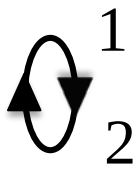
New Method for Calculating the One-Particle Green's Function with Application to the Electron-Gas Problem*

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

Approximate vertex function (I)

We stay within the approximation: $\Gamma(1,2,3) = \delta(1,2)\delta(1,3)$

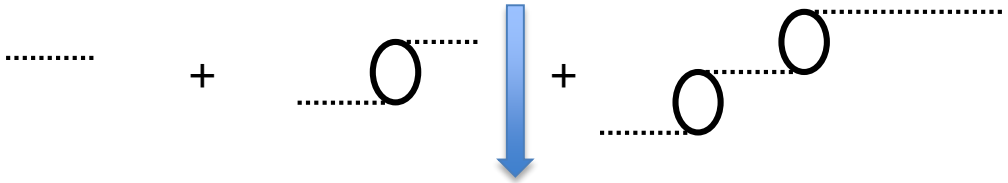
The polarization propagator is a particle-hole one:



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

W is the bare interaction plus an induced interaction which includes RPA correlations (attractive/repulsive)

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



G. Gori et al., Phys. Rev C 72, 011302(R) (2005)

$$M(1,2) = iG(1,2)W(3,2)$$

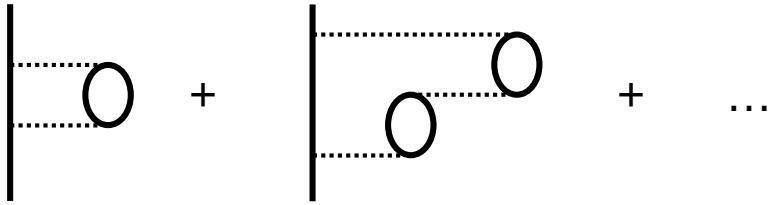
$$G(1,2) = G^0(1,2) + G^0(1,3)M(3,4)G(4,2)$$

Approximate vertex function (II)

L. Schiacchitano, M.Sc. Thesis, University of Milano (unpublished); M. Baldo *et al.*, J. Phys. G 42 (2015) 085109.

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

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



$$M(1,2) = iG(1,2)W(3,2)$$

Self-energy with the RPA correlations associated with W

Dyson equation

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

Iterative solution

$$M \longrightarrow G \longrightarrow \Gamma \longrightarrow \Pi \longrightarrow W$$

Order 0

$$M = 0$$

$$G = G^0$$

$$\Gamma = 1$$

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

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

Order 1

$$M = iG^0W$$

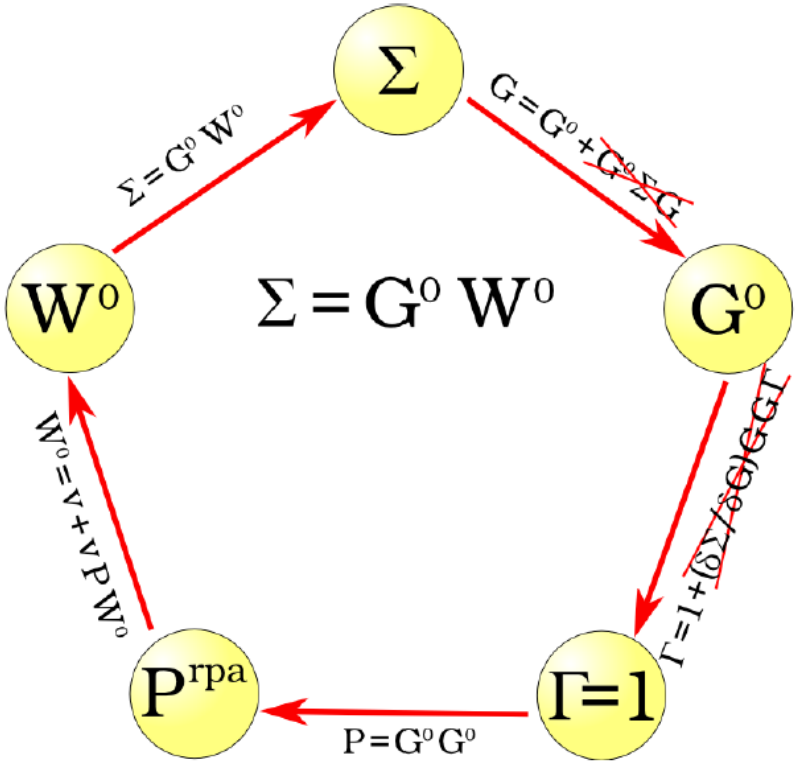
$$G = G^0 + G^0MG$$

$$\Gamma = 1$$

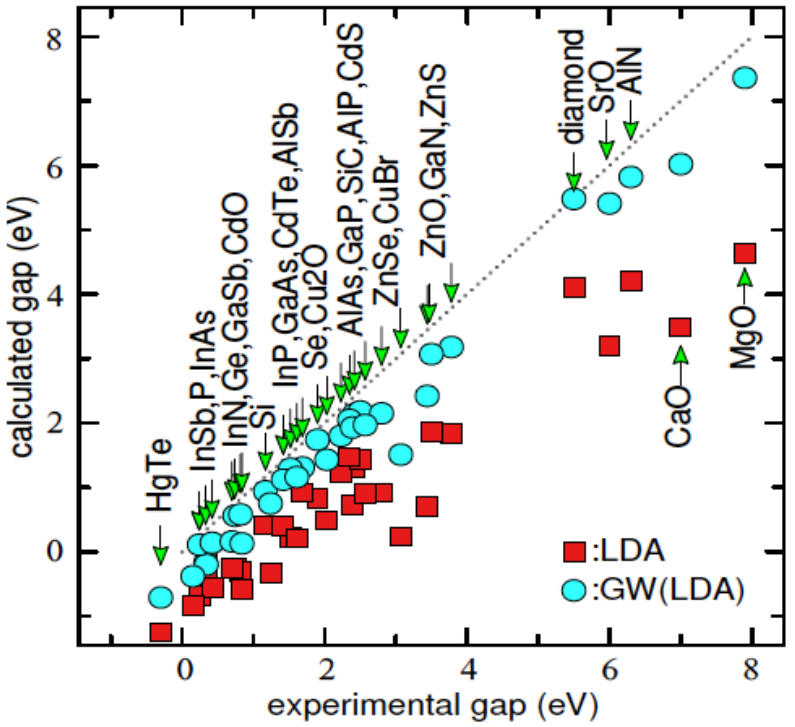
$$\Pi = -iGG$$

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

Hedin's pentagon: possible strategy



Courtesy of F. Sottile



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

What we have done so far (I)

$$M = iG^0 W$$

$$G = G^0 + G^0 M G$$

$$\Gamma = 1$$

$$\Pi = -iGG$$

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

This M is the one of the “traditional” particle-vibration coupling approach (PVC).

Particle-vibration coupling

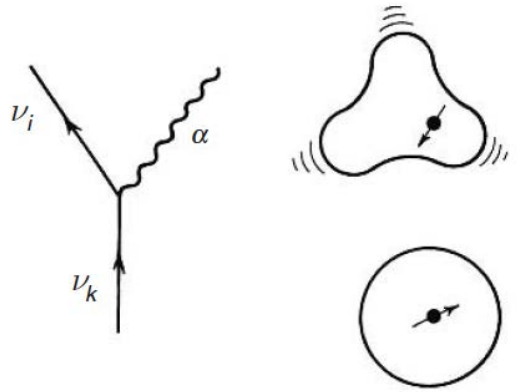
- The basic idea is that in spherical nuclei there are **single-particle states** and (mainly surface) **collective vibrations**. The spectra result from their **interplay.**

- Deformed nuclei: particle-rotation coupling.

- **Adiabatic approximation in general not valid**.

- In the past, phenomenological models based on the experimental properties of the vibrations ("phonons"): Nuclear Field Theory or NFT (Copenhagen), Quasiparticle-phonon model or QPM (Dubna).

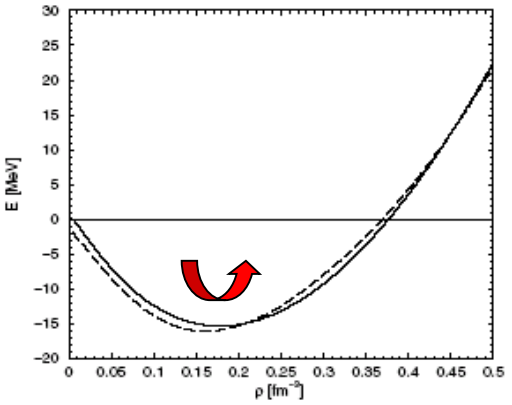
	$E(I)$ [MeV]		$B\left(\frac{E}{M}\right)I$ $[e^2\,\mathrm{fm}^{2I}]$ $[\mu^2\,\mathrm{fm}^{2I-2}]$	
	theory	exp	theory	exp
3^-	2.63	2.61	546	$540 \pm 30 \times 10^3$
5^-	3.39	3.19	285	$462 \pm 55 \times 10^6$
5^-	3.82	3.71	301	330×10^6
2^+	4.49	4.07	3070	2965
4^+	4.69	4.32	757	1287×10^4
6^+	4.77	4.42	210	230×10^8
1^+	7.50	7.56	568	5.9
1^+	8.30	7.99	11.00	10.0
2^-	7.51		11.00×10^3	



RPA for collective vibrations

$$E = \langle \Psi | \hat{H} | \Psi \rangle = \langle \Phi | \hat{H}_{eff} | \Phi \rangle = E[\hat{\rho}]$$

$|\Phi\rangle$ **Slater determinant** $\Leftrightarrow$ $\hat{\rho}$ **1-body density matrix**



- Within a time-dependent theory (TDKS), one can describe harmonic oscillations around the minimum.
- The restoring force is: $v \equiv \dfrac{\delta^2 E}{\delta \rho^2}$.
- The linearization of the equation of the motion leads to RPA[1].

[1]Random Phase Approximation.

$$X_{\mathrm{ph}} |ph^{-1}\rangle - Y_{\mathrm{ph}} |hp^{-1}\rangle$$

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

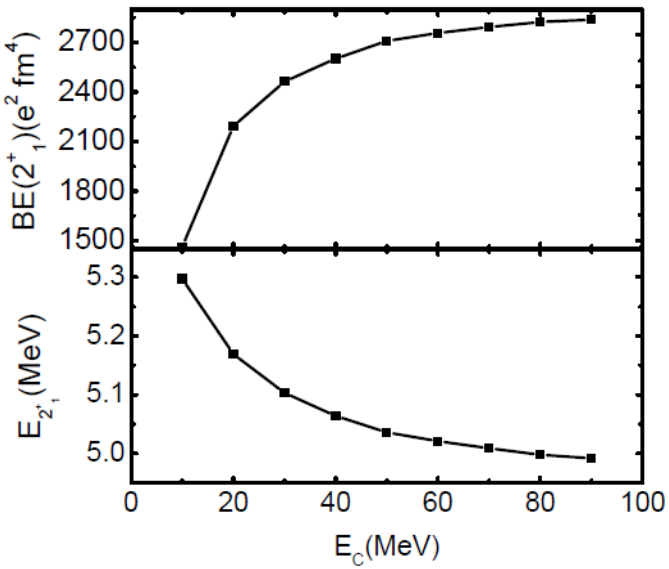
Our implementation

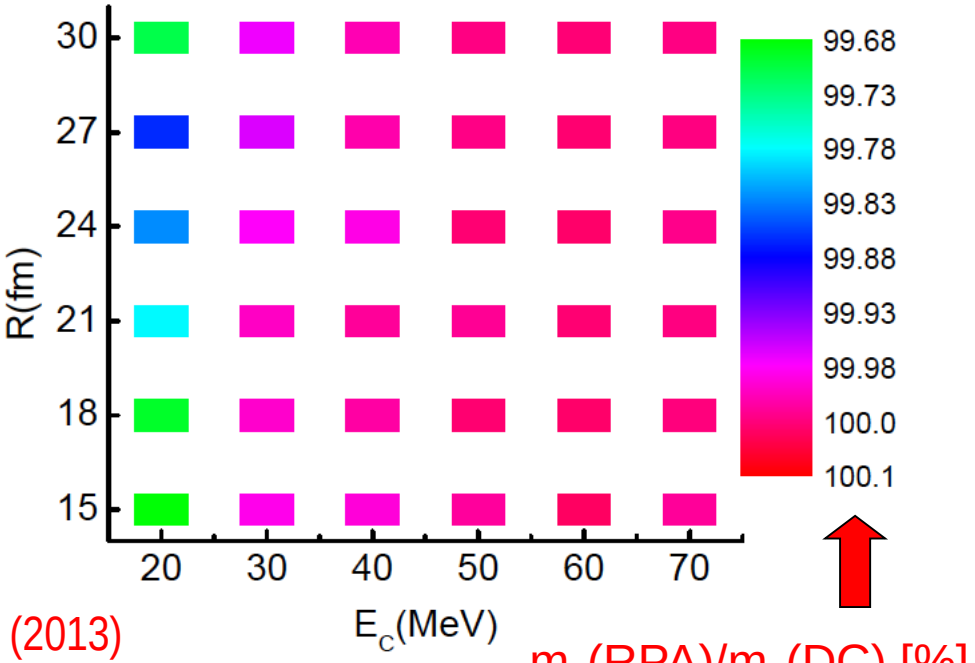
The continuum is discretized. We define a p-h basis and then the RPA matrix on this basis is diagonalized. Parameters: R, E_C.

The energy-weighted sum rule should be equal to the double-commutator value: well fulfilled !

$$m_1(\hat{O}) = \sum_\nu E_\nu |\langle \nu|\hat{O}|\tilde{0}\rangle|^2 = \frac{1}{2}\langle 0|[\hat{O},[H,\hat{O}]]|0\rangle$$

^{208}Pb - SGII





m_1(RPA)/m_1(DC) [%]

G.C. *et al.*, Computer Physics Commun. 184, 142 (2013)

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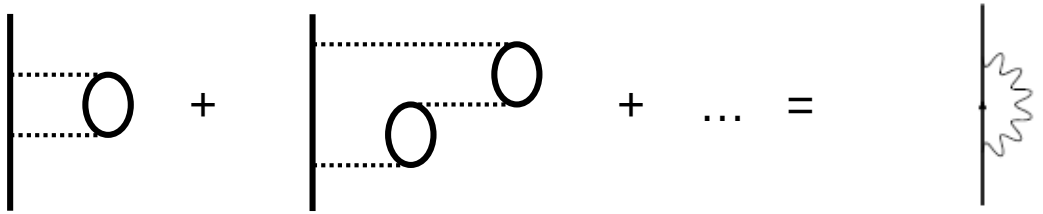
Second order approximation



$$M = iG^0W$$

One first calculates the vibrations within linear response theory (RPA).

The above diagram is calculated by selecting collective vibrations (in some cases, one attempts at solving the problem of the Pauli principle violation).

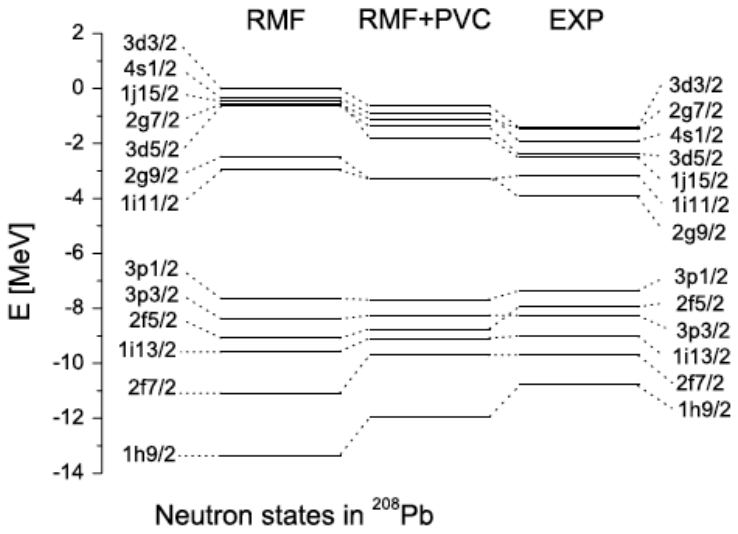
$$M_i(\omega) = \frac{1}{2j_i+1}\left(\sum_{nL,\ p>F}\frac{|\langle i||V||p,nL\rangle|^2}{\omega-\varepsilon_p-\omega_{nL}+i\eta}+\sum_{nL,\ h<F}\frac{|\langle i||V||h,nL\rangle|^2}{\omega-\varepsilon_h+\omega_{nL}-i\eta}\right)$$

Currently, calculations without uncontrolled approximations are possible.

Second order perturbation theory : $\varepsilon = \varepsilon^{(0)} + M(\varepsilon)$.

Self-consistent results for ^{208}Pb

RMF-NL3



E. Litvinova *et al.*, Phys. Rev. C73, 044328 (2006).

R.m.s. deviation experimental vs. theoretical energies (Skyrme-T44)

HF	1.42 [MeV]
PVC (central)	1.00
PVC (including spin-orbit)	0.91
PVC (including tensor)	0.87

Effective mass m*/m

HF	0.84
PVC (central)	0.97
PVC (including spin-orbit)	1.00
PVC (including tensor)	1.04

L. Cao *et al.*, Phys. Rev. C82, 1 (2010).

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What we have done so far (II)

$$M = iG^0 W$$

$$G = G^0 + G^0 M G$$

$$\Gamma = 1$$

$$\Pi = -iGG$$

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

One can go beyond perturbation theory, solving the Dyson equation.
This has been done with proper continuum treatment.
PRC 86, 034318 (2012).

Dyson equation in the continuum

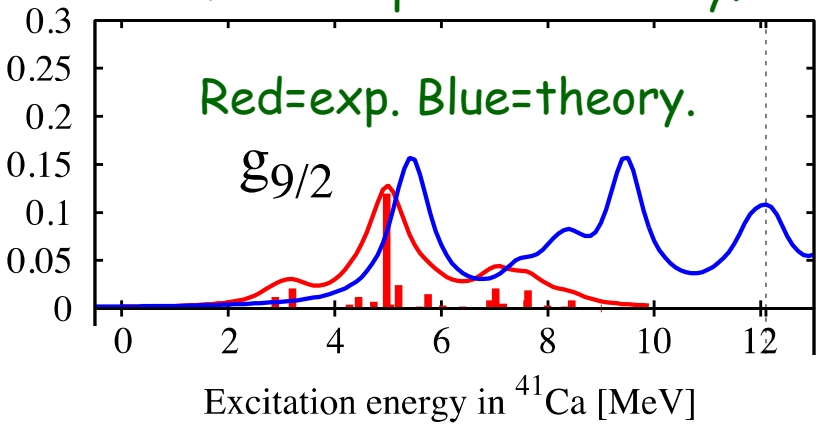
Coordinate space representation

$$M(\omega) =$$

$$G = G^0 + G^0 M G$$

$$S = -\frac{1}{\pi}\int d^3r\; G(\vec{r},\vec{r};\omega)$$

Y-axis: spectral density.



K. Mizuyama, GC, and E. Vigezzi, PRC 86, 034318 (2012).

APPLICATION TO SCATTERING

K. Mizuyama, K. Ogata, PRC 86, 041603(R)

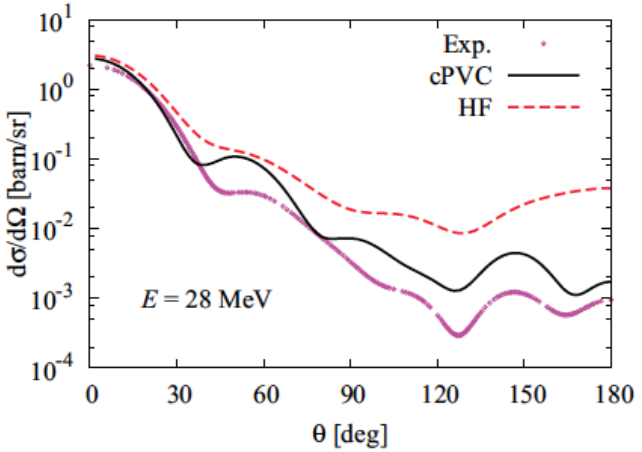


FIG. 5. (Color online) Angular distribution of the neutron elastic cross section by ^{16}O at 28 MeV. The solid (dashed) line shows the result of the cPVC method (HF calculation). Experimental data are taken from Ref. [19].

What we have done so far (IV)

$$M = iG^0 W$$

$$G = G^0 + G^0 M G$$

$$\Gamma = 1$$ ← Frozen

$$\Pi = -iGG$$

$$W = \kappa + \kappa \Pi W$$ ← RPA plus PVC

RPA plus PVC

$$\begin{pmatrix} A+M(\omega) & B \\ -B & -A-M^*(-\omega) \end{pmatrix}$$

$$M_{\mathrm{ph,p'h'}}(\omega) = \sum_{\alpha} \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{\omega-\omega_\alpha+i\eta}$$

The state α is 1p-1h plus one "phonon".

The scheme is known to be effective to account for the spreading width of GRs.

$$\Pi = -iGG$$

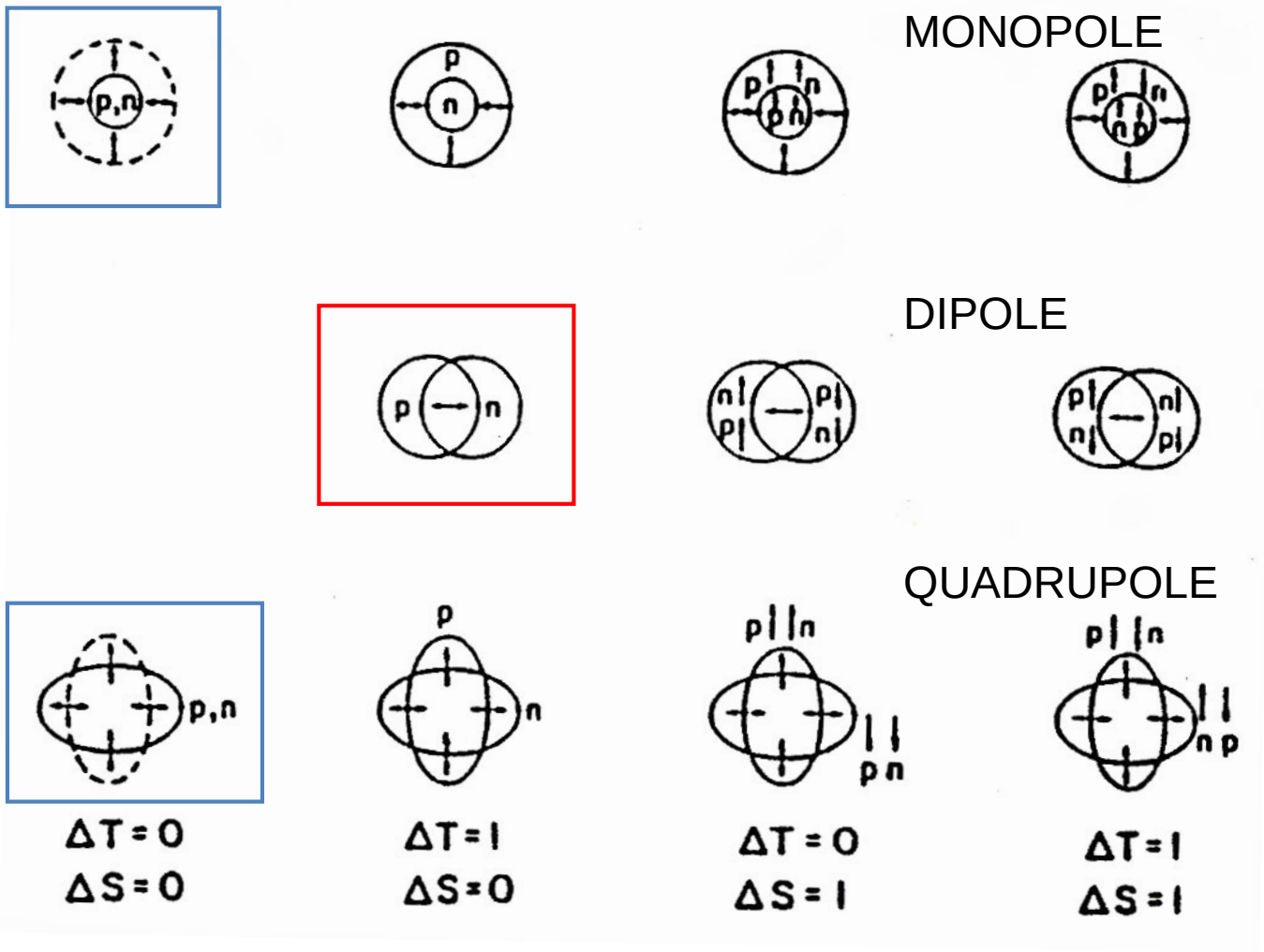
$$W = \kappa + \kappa\Pi W$$

h'

Nuclear collective modes

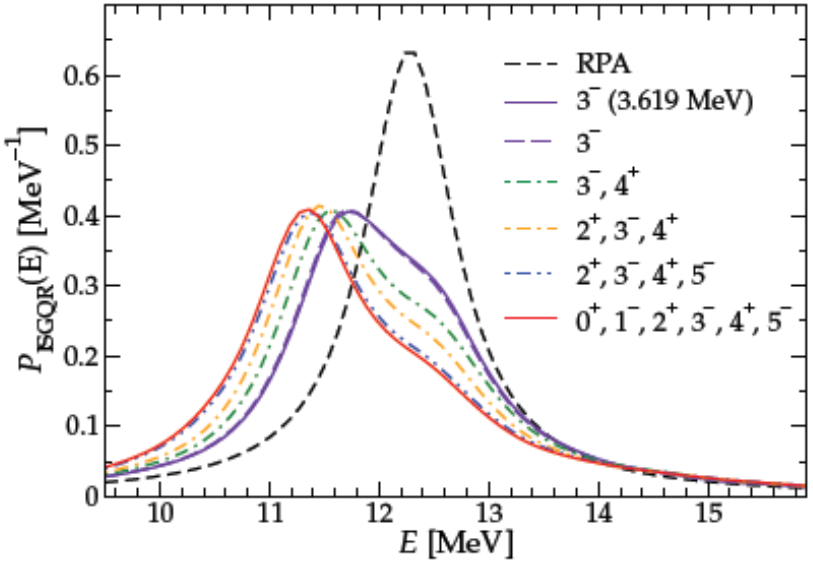
In the isoscalar resonances, the n and p oscillate in phase

In the isovector case, the n and p oscillate in opposition of phase



The quadrupole response in ^{208}Pb

- Isoscalar (*PRC* **85**, 014305 (2012))

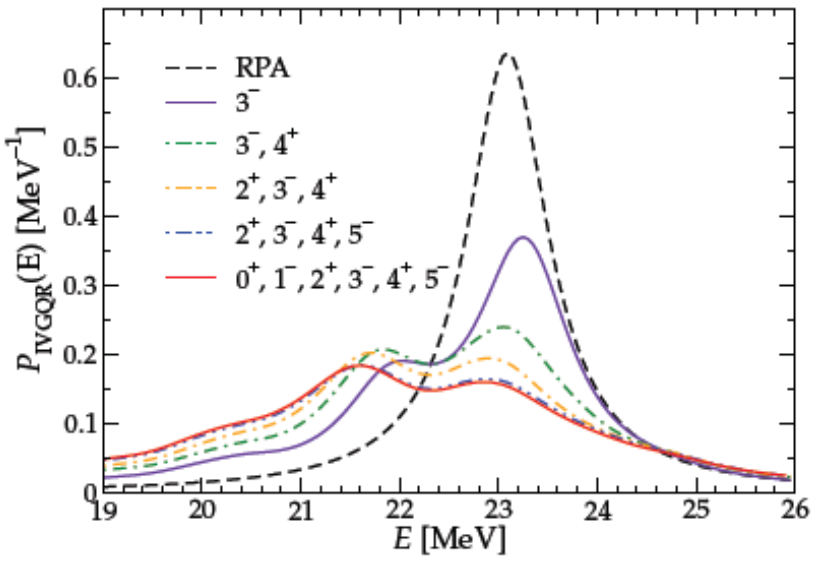


$E_{ISGQR} = 11.3$ MeV $\quad (10.9 \pm 0.3$ MeV$)$

$\Gamma_{ISGQR} \approx 2.3$ MeV $\quad (3.0 \pm 0.3$ MeV$)$

Exp. *PRC* **69**, 034315 (2004)

- Isovector (*PRC* **87**, 034301 (2013))

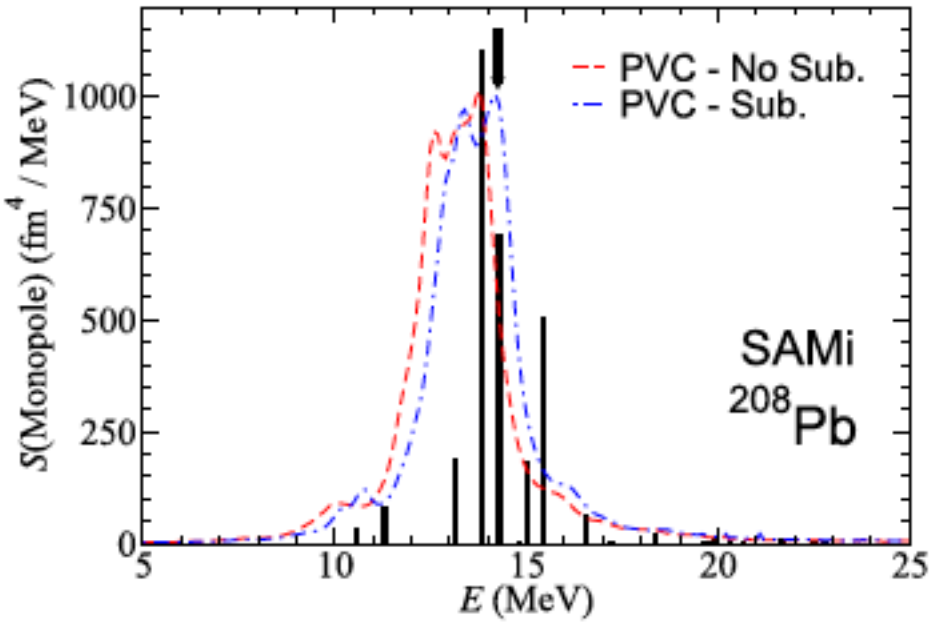


$E_{IVGQR} = 22.0$ MeV $\quad (20.2 \pm 0.5$ MeV$)$

$\Gamma_{IVGQR} \approx 4$ MeV $\quad (5.5 \pm 0.5$ MeV$)$

Exp. *PRL* **68**, 3507 (1992)

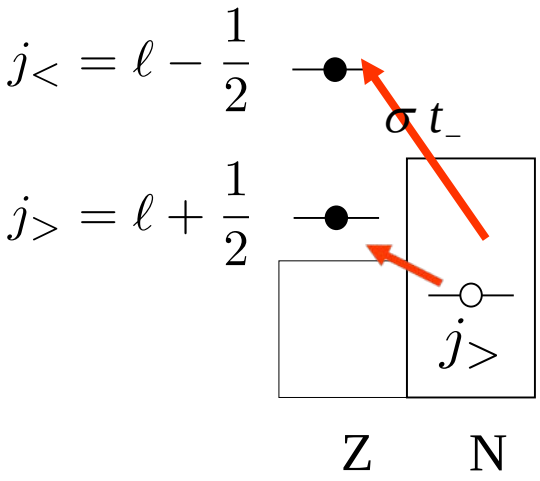
The monopole resonance in ^{208}Pb

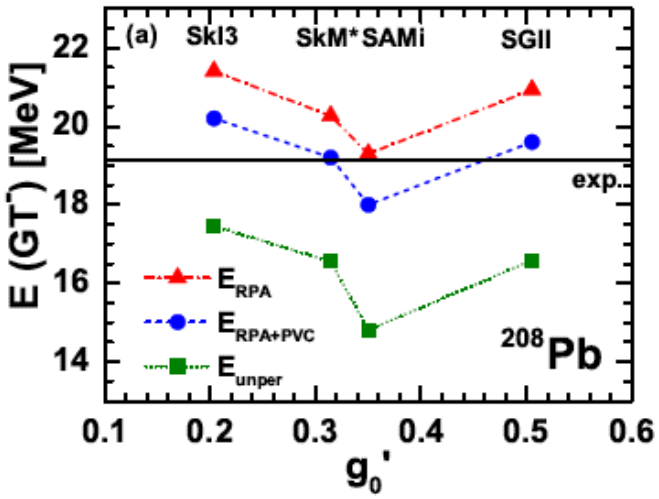


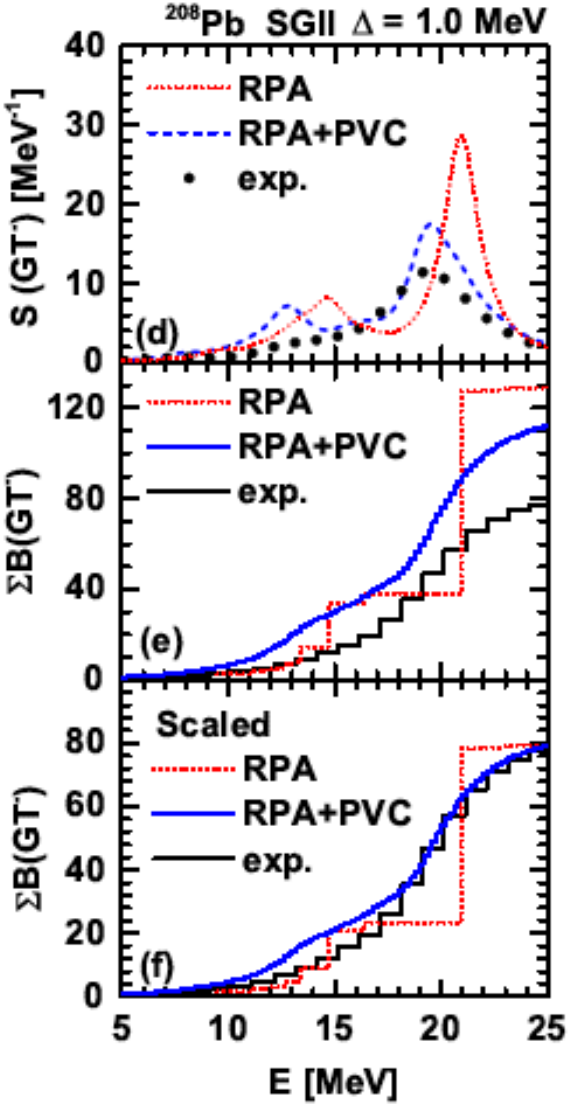
X. Roca-Maza *et al.*, J. Phys. G 44 (2017) 044001.

$$M(\omega) \rightarrow M(\omega) - M(\omega = 0)$$

Charge-exchange states







- The energy shift induced by PVC is very weakly interaction-dependent.
- The PVC calculations reproduce the lineshape of the GT response quite well.

Cf. talk by Y. Niu

Conclusions

- DFT problem in nuclear physics: successful approach.
- Yet, we lack some of the rigorous results that exist for Coulomb systems.
- Mapping of more fundamental approaches to DFT should be pushed.
- There is debate about the functional(s) for collective excitations, single-particle excitations (large amplitude motion not discussed in this talk).
- Matching many-body Green's function theory and DFT also is still in its infancy.
- Main question: at which level should we fit the EDF parameters ?

- G. Accorto, P.F. Bortignon, L. Capelli, A. Rancati, D. Rizzo, X. Roca-Maza, R. Romano, L. Sciacchitano, E. Vigezzi (Milano)
- M. Baldo (INFN Catania, Italy)
- M. Grasso, N. Van Giai (IPN Orsay, France)
- Y. Niu (ELI Nuclear Physics, Romania)
- J. Meng (PKU, China)
- L. Cao (NCEPU, Beijing, China)
- C.L. Bai (Sichuan University, Chengdu, China)
- H. Sagawa (RIKEN and U. Aizu, Japan)
- K. Mizuyama (RCNP, Japan)