A unified approach for nuclear excitations





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Nuclear Density Functional Theory (DFT)

 $E = \left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle = \left\langle \Phi \middle| \hat{H}_{eff} \middle| \Phi \right\rangle = E[\hat{\rho}]$ $|\Phi\rangle \text{ Slater determinant } \Leftrightarrow \hat{\rho} \text{ 1-body density matrix}$

- The Hohenberg-Kohn (HK) theorem guarantees that "the" exact functional exists but gives no clue on how to build it.
- One can start from a force V_{eff} and write $H_{eff} = T + V_{eff}$. E is the expectation value on a general Slater determinant.
- $\delta E = 0$ provides Hartree-Fock or Kohn-Sham (integro-)differential equations
- Another possibility is to write directly the functional E[ρ] and fit the parameters to the data.

 $E=a\rho^2 + \dots$ (can become involved)



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Modern functionals and their performance

- They are as "fundamental" as other models because of the **HK** • theorem.
- They are applicable to almost the whole isotope chart and to excited • states.
- Typical number of parameters \sim 10.
- Error on masses of the order of 1 MeV (can go further down).
- Trends of charge radii and deformations fairly well reproduced.
- Good description of excitations such as giant resonances, rotational bands.
- They can also be applied to β and $\beta\beta$ transitions.
- There is current interest in large • amplitude motion, reactions etc.

(...)



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A specific open questions is whether pairing is properly included in current EDFs (not only between equal particles but also between p and n).

H. Sagawa, C.L. Bai, GC, Phys. Scr. 91, 083011 (2016)

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

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Beyond the simple DFT

There are phenomena or observables that are outside the DFT framework.

The solution of the Kohn-Sham equations provides s.p. orbitals that are not the observed states in the A+1 or A-1 nuclei.

Single-particle strength 9/2⁺ strength in ⁴¹Ca.



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



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Multipole strength Gamow-Teller strength in ⁶⁰Ni



Goal and strategy

- We would like to have an effective theory that is based on s.p. and collective states that comes from DFT but also includes their mutual coupling.
- It might be solved at given order.
- It should provide the fragmentation of states that characterizes the low-energy spectra, and the broad features in the giant resonance region.





Particle-vibration coupling (PVC) - I

In spherical nuclei this is the most effective way, if not the only one, to explain **fragmentation and widths** of single-particle and giant resonances in a consistent fashion. Valid both at the ~1 MeV and ~10 MeV scales.





Particle-vibration coupling (PVC) - II

A formal description of the model can be given.

One starts from the Hedin's equations, that involve

 $G, \Sigma, W, \Pi, \Gamma$

and performs a series of approximations.

Particle-Vibration Coupling (PVC). M. Baldo *et al.*, J. Phys. G: Nucl. Part. Phys. 42 (2015) 085109. Cf. I. Hamamoto, V. Soloviev *et al.*, V. Tselyaev, E. Litvinova *et al.* [...]





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Focus

1. New model for odd-nuclei

HCM (Hybrid configuration mixing)

2. Extension of the model for GRs and β -decay: inclusion of T=1 and T=0 pairing

Q R P A + Q P V C (Quasiparticle Random Phase Approximation plus quasiparticle-vibration coupling)





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Towards complete spectroscopy of odd nuclei

• There are several examples of spectra in which "particle" states (large spectroscopic factor in transfer reactions) coexist with states made up with "particle plus core vibration" states (gamma decay similar to that of the core vibration).

$$B(E\lambda, [j' \otimes \lambda]_j \to j') = B(E\lambda, \lambda \to 0)$$

- Could be a good playground for particle-vibration coupling models ...
- ... but in some cases particle-phonon states are instead 2p-1h, or 3p-2h states ("shell model-like" states).





Hybrid Configuration Mixing (HCM) model - I

We start from a **basis** made up with **particles** (or holes) around a core, and with **excitations** of the same core (RPA "phonons").





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Hybrid Configuration Mixing (HCM) model - II

- Some of the RPA phonons might be actually pure p-h states. Then, the states of our basis are 2p-1h. In this sense they are not "vibrations" and the model cannot be considered "PVC".
- In this case Pauli principle violations can be important. We correct for the non-orthonormality and overcompleteness of the basis by introducing the NORM matrix.

$$n(j_1'n_1J_1, j_2'n_2J_2) = \delta(j_1', j_2')\delta(n_1, n_2)\delta(J_1, J_2) - \sum_{h_1} (-)^{J_1 + J_2 + j_1' + j_2'} \hat{J}_1 \hat{J}_2 \left\{ \begin{array}{cc} j_2' & j_{h_1} & J_1 \\ j_1' & j & J_2 \end{array} \right\} X_{j_2'h_1}^{(n_1J_1)} X_{j_1'h_1}^{(n_2J_2)}$$

This is the overlap between 1p-1 "phonon" states. The diagonal part reduces to $1 - (2j+1)^{-1}$ in simple cases.

$$\mathcal{H} - E\mathcal{N} = 0$$



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Basic equation (cf. SM and/or GCM)

$$\mathcal{H} - E\mathcal{N} = 0$$

$$\mathcal{H} = \begin{pmatrix} \varepsilon_{n_{1}lj} & 0 & \frac{\langle n_{1}lj||V||n'_{1}l'_{1}j'_{1}N_{1}J_{1} \rangle}{\hat{j}} & \frac{\langle n_{1}lj||V||n'_{2}l'_{2}j'_{2}N_{2}J_{2} \rangle}{\hat{j}} \\ 0 & \varepsilon_{n_{2}lj} & \frac{\langle n_{2}lj||V||n'_{1}l'_{1}j'_{1}N_{1}J_{1} \rangle}{\hat{j}} & \frac{\langle n_{2}lj||V||n'_{1}l'_{1}j'_{1}N_{1}J_{1} \rangle}{\hat{j}} & \frac{\langle n_{2}lj||V||n'_{1}l'_{1}j'_{1}N_{1}J_{1} \rangle}{\hat{j}} \\ \frac{\langle n_{1}lj||V||n'_{2}l'_{2}j'_{2}N_{2}J_{2} \rangle}{\hat{j}} & \frac{\langle n_{2}lj||V||n'_{2}l'_{2}j'_{2}N_{2}J_{2} \rangle}{\hat{j}} & \varepsilon_{n'_{1}l'_{1}j'_{1}} + \hbar\omega_{N_{1}J_{1}} & 0 \\ \end{pmatrix} \\ \mathcal{N} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & \dots \\ 0 & 1 & \dots & 0 & 0 & \dots \\ 0 & 1 & \dots & 0 & 0 & \dots \\ 0 & 0 & \dots & n(j'_{1}n_{1}J_{1}, j'_{1}n_{1}J_{1}) & n(j'_{1}n_{1}J_{1}, j'_{2}n_{2}J_{2}) & \dots \\ 0 & 0 & \dots & n(j'_{2}n_{2}J_{2}, j'_{1}n_{1}J_{1}) & n(j'_{2}n_{2}J_{2}, j'_{1}n_{1}J_{1}) & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$



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Results for ⁴⁹Ca



The spectrum is **more stretched** in theory than in experiment; nonetheless, the **agreement is quite good**.



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Electromagnetic transition probabilities



In the transition between two states made up with particle plus phonon, the electromagnetic operator (red dot) can act either on the particle or on the p and h that compose the phonon.



Results for ¹³³Sb

15/2⁻.

SkX

Only 2^+ , 3^- and 4^+ core excitations are genuine "phonons". There are more core excitations in the model space, and they are 1p-1h (mainly $h_{11/2}^{-1}-f_{7/2}$). 6+ has 2-3 components.

The spectrum includes particle-phonon states as well as 2p-1h states.

5 Energy [MeV .21/2+17/2+15/2+11/2+2+_11/2-_3/2+ • New measurements (G. Bocchi et al.) have shed light on some **HIGHER SPIN** states. $B(M1, 15/2^+ \rightarrow 13/2^+) = 0.24 \text{ W.u.}$ $B(M1, 13/2^+ \rightarrow 11/2^+) = 0.004 \text{ W.u.}$ Core excitation Results Experiment

The r.m.s. deviation th.-exp. is **0.869 MeV**.

It drops to 0.246 MeV if we exclude the 13/2⁻,

(ratio = 60; theory provides a ratio of 20).



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5/2 +7/2-

A similar model for resonances: RPA plus particle-vibration coupling

$$\begin{array}{c} A + \Sigma(E) & B \\ -B & -A - \Sigma^*(-E) \end{array} \right) \qquad \Sigma_{\rm php'h'} (A)$$

One first solves self-consistent Hartree-Fock plus Random Phase Approximation (HF-RPA).

One adds the self-energy contribution (the state α is 1p-1h plus one phonon).

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



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Extension to the case of open-shell nuclei

The basis is made up with states from **full HFB**. In the case of zero-range interactions, at a given cut-off for E_{qp} the pairing gap is fitted.

Phonons are from **quasi-particle RPA** (QRPA). We select the collective ones.

The scheme is fully self-consistent also in the pairing channel.





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• p-h channel : Skyrme

$$V^{T=1}(\vec{r}_1,\vec{r}_2)=\hat{P}_sV_0\delta\left(\vec{r}_1-\vec{r}_2
ight)$$



• p-p channel : IS and IV pairing (cf. the talk by H. Sagawa) $V^{T=0}(\vec{r_1}, \vec{r_2}) = \hat{P}_t f V_0 \delta(\vec{r_1} - \vec{r_2})$

Test and performance of the model

• Isospin invariance: $V_{\rm C} = 0 \implies [H, \vec{T}] = 0 \implies E_{\rm IAS} = 0$

 $E_{IAS}(QRPA) = 280 \text{ keV}, \quad E_{IAS}(QRPA+QPVC) = 200 \text{ keV} \quad [^{78}Ni - SkM^*]$

• <u>2⁺ in ¹²⁰Sn:</u>

 $E_x = 1.42 \text{ MeV}$ (exp. 1.17 MeV), $B(E2) = 2632 \text{ e}^2\text{fm}^4$ (exp. 2016 e^2fm^4)



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Charge-exchange transitions

- Some transitions may be inside the allowed β -decay window.
- However, most of them require external energy so that they are induced by charge-exchange reactions, like (p,n) or (³He,t). We look at GTR.

The study of their properties can greatly improve our knowledge of the charge-changing part of H_{nucl} or $E[\rho]$.



At the same time the matrix elements of the transitions involved in double- β decays must be known to extract the neutrino mass (cf. J. Menéndez).





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GTR in ²⁰⁸Pb



Y. Niu *et al.,* PRC 90, 054328 (2014).

- The energy shift induced by PVC is very weakly interaction-dependent.
- The PVC calculations reproduce the lineshape of the GT response quite well.
- Part of the experimentally observed quenching is accounted for.



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QRPA plus PVC: results for ¹²⁰Sn



- Theory reproduces the data in the high-energy GTR region.
- Not enough quenching.

NFN

• The effect of T=0 pairing is not large but it goes in the right direction of improving the agreement with experimental data.



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Particle-vibration effect on β -decay

PVC can strongly affect the half-lives:

$$T_{1/2} = \frac{D}{g_A^2 \int_{E_c}^{Q_\beta} S(E) f(Z, E) dE}$$

Its effect is to fragment and shift down the RPA peaks, so that there is more strength in the decay window. The effect is enhanced by the phasespace factor. We definitely improve agreement with experiment.



The case of open-shell isotopes: ^ANi



- The effect is confirmed in open-shell isotopes, where QRPA+QPVC provides much better agreement with experiment than simple QRPA.
- Weak sensitivity to T=0 pairing in this case.



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β-decay of ¹⁰⁰Sn

Superallowed Gamow–Teller decay of the doubly magic nucleus ¹⁰⁰Sn Nature 486, 341 (2012)



Figure 6 | Log(ft) values of allowed nuclear β -decays. Number distribution of log(ft) values for allowed β -transitions (obeying the selection rules). The data are from ref. 26. The values are for generally allowed Gamow–Teller transitions between 0⁺ and 1⁺ states (black), mixed Fermi/Gamow–Teller transitions (blue) and the well-established pure, superallowed Fermi transitions from 0⁺ to 0⁺ states (green). The decay of ^{frog}Sn is unique because it has the smallest known log(ft) value (red) of any nuclear β -decay.



NFN

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t _{1/2}	
RPA RPA+PVC	17.41 s 4.18 s
Exp.	1.11 s

Co-workers

- <u>G. Bocchi</u>, P.F. Bortignon, M. Brenna, X. Roca-Maza, E. Vigezzi (University of Milano, Italy)
- <u>Y. Niu</u> (ELI, Magurele, Romania)
- J. Meng (PKU, Beijing, China)
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- C.L. Bai (Chengdu, China)
- H. Sagawa (RIKEN, Japan)
- Z. Niu (iTHES, RIKEN, Japan)



I N F N



Conclusions

- Density Functional Theory is a powerful framework to describe many properties of atomic nuclei.
- There are nonetheless properties outside the DFT framework, and we are interested in extending DFT in order to reproduce them.
- A clear physical case: states with mixed particle and phonon character in odd nuclei, with their electromagnetic transitions.
- We also have (Q)RPA+(Q)PVC for GRs.
- Applied to GTRs, our model accounts for most of the width and part of the quenching. It also improves significantly the description of β -decay. We now deal with open-shell systems.





Backup slides



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Skyrme vs. relativistic functionals

Skyrme forces are widely used: they generate LOCAL functionals.

$$\hat{u}_{\text{Sk}}(r_{12}) = t_0(1+x_0\hat{P}_{\sigma})\delta(r_{12}) + \frac{1}{2}t_1(1+x_1\hat{P}_{\sigma})(\hat{k}^{\dagger 2}\delta(r_{12}) + \delta(r_{12})\hat{k}^2) \\
+ t_2(1+x_2\hat{P}_{\sigma})\hat{k}^{\dagger} \cdot \delta(r_{12})\hat{k} + \frac{1}{6}t_3(1+x_3\hat{P}_{\sigma})\delta(r_{12})\rho^{\alpha}\left(\frac{r_1+r_2}{2}\right) \\
+ iW_0(\hat{\sigma}_1+\hat{\sigma}_2) \cdot \hat{k}^{\dagger} \times \delta(r_{12})\hat{k}.$$
short-range repulsion

In the covariant models the nucleons are described as Dirac particles that exchange effective mesons. One starts from Lagrangians.

$$\mathcal{L}_{int} = -\bar{\psi}\Gamma_{\sigma}\sigma\psi - \bar{\psi}\Gamma^{\mu}_{\omega}\omega_{\mu}\psi - \bar{\psi}\vec{\Gamma}^{\mu}_{\rho}\vec{\rho}_{\mu}\psi - \bar{\psi}\Gamma^{\mu}_{e}A_{\mu}\psi$$

$$\Gamma_{\sigma} = g_{\sigma}, \quad \Gamma^{\mu}_{\omega} = g_{\omega}\gamma^{\mu}, \quad \vec{\Gamma}^{\mu}_{\rho} = g_{\rho}\vec{\tau}\gamma^{\mu}, \quad \Gamma^{\mu}_{e} = e\frac{1-\tau_{3}}{2}\gamma^{\mu}$$



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Fragmentation of s.p. strength



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APPLICATION TO SCATTERING Courtesy: K. Mizuyama



workshop on microscopic theories of nuclear structure and dynamics



Neutrons plus a ⁴⁸Ca vibration ?



⁶⁴Ni+⁴⁸Ca (5.7 MeV/u) performed at LNL recently.

The angular momenta have been found to be aligned <u>perpendicular</u> to the reaction plane. <u>Spin</u> and lifetimes extracted.



Spectroscopy of ¹³³Sb (¹³²Sn + p)

 Despite the importance of the region around ¹³²Sn, the information about low-lying states of neighbouring nuclei need still be completed.

17/2+ 21/2+ T-16.6(3) µs 4545(10) 4526.3 15/2+ 4464.6 4302.0 167.7 13/2 166.1 15/2 2 4360.2 4297.0 110.2 $11/2^{+}$ 4191.8 1505.3 $11/2^{-}$ 2791.7 4297 (4191 8 1829.5 5/2+ 962.1 962.1 7/2+

W. Urban *et al.*, PRC 79, 037304 (2009)

- Recently new measurements (G. Bocchi et al.) have shed light on some HIGHER SPIN states (up tp 25/2⁺).
 B(M1, 15/2⁺→13/2⁺) = 0.24 W.u.
 B(M1, 13/2⁺→11/2⁺) = 0.004 W.u.
 (ratio = 60; theory provides a ratio of 20).
- The odd proton is $g_{7/2}$. Low spin states may come from coupling to 2⁺, 3⁻, 4⁺ phonons. High spin states can only come from $g_{7/2}$ coupled to $h_{11/2}$ ⁻¹ $f_{7/2}$ neutron p-h states.



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Electromagnetic transitions and the mutable nature of the wavefunction



red:
$$\pi g_{9/2} \otimes 2^+, 4^+$$

blue: $\pi g_{9/2} \nu h_{11/2}^{-1} \nu f_{7/2}$

This nature is reflected in the M1 transition probabilities.

The wave functions of $15/2^+$ and $13/2^+$ are dominated by $g_{9/2}$, $h_{11/2}^{-1} f_{7/2}$, so the B(M1) transition is made up with s.p. amplitudes. B(M1)_{th} = 0.021 W.u.

In the case of the transition $13/2^+ \rightarrow 11/2^+$, the final state has phonon component so there is a mismatch in the components and B(M1) is quenched, B(M1)_{th} = 0.001 W.u. Ratio = 20.



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Microscopic content of the states

EXP. Calculation with 2^+ , 3^- , 4^+

All excitations below 5.5 MeV included

$9/2^{+}$	4.027	$3.84 \ [\pi g_{7/2} \otimes 2^+ \ (0.82)]$	$4.08 \ [\pi g_{7/2} \otimes 2^+ \ (0.80)]$
$11/2^{+}$	4.192	$3.82 \ [\pi g_{7/2} \otimes 2^+ \ (0.74)]$	4.11 $[\pi g_{7/2} \otimes 2^+ (0.78)]$
$13/2^{+}$	4.302	4.66 $[\pi g_{7/2} \otimes 4^+ (1.00)]$	4.44 $\left[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (0.40)\right]$
$15/2^{+}$	4.464	$4.37 \ [\pi g_{7/2} \otimes 4^+ \ (0.98)]$	4.45 $[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (0.40)]$
$17/2^{+}$	4.526		4.58 $[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (0.66)]$
$19/2^{+}$	4.539		4.64 $\left[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (0.73)\right]$
$21/2^+$	4.545		4.76 $[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (0.92)]$
$23/2^+$	4.753		4.83 $[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (0.98)]$
$25/2^+$	4.844		5.11 $[\pi g_{7/2} \nu h_{11/2}^{-1} \nu f_{7/2} (1.00)]$



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Different kinds of excitations in ¹³²Sn

	Energy		Transi	tion strength	Main components
	Exp.	Theory	Exp.	Theory	Theory
		(RPA)		(RPA)	(RPA)
2+	4.041	3.87	7	4.75	$\nu h_{11/2}^{-1} f_{7/2} (0.56), \pi g_{9/2}^{-1} d_{5/2} (0.19), \pi g_{9/2}^{-1} g_{7/2} (0.14)$
3-	4.352	5.02	> 7.1	9.91	$\nu s_{1/2}^{-1} f_{7/2} (0.40), \nu d_{3/2}^{-1} f_{7/2} (0.12), \pi p_{1/2}^{-1} g_{7/2} (0.12)$
4+	4.416	4.46	4.42	5.10	$\nu h_{11/2}^{-1} f_{7/2} (0.63), \pi g_{9/2}^{-1} g_{7/2} (0.21)$
6^{+}	4.716	4.73		1.65	$\nu h_{11/2}^{-1} f_{7/2} (0.86), \pi g_{9/2}^{-1} g_{7/2} (0.11)$
4-	4.831	5.68		0.16	$\nu s_{1/2}^{-1} f_{7/2} (0.91)$
8+	4.848	4.80		0.28	$\nu h_{11/2}^{-1} f_{7/2} (0.98)$
5^{+}	4.885	4.77		0.61	$\nu h_{11/2}^{-1} f_{7/2} (0.99)$
7^{+}	4.942	4.80		0.81	$\nu h_{11/2}^{-1} f_{7/2} (0.98)$
5^{-}	4.919	5.98		0.96	$\nu d_{3/2}^{-1} f_{7/2} (0.96)$
(9^+)	5.280	4.99		0.16	$\nu h_{11/2}^{-1} f_{7/2} (0.99)$
2^{-}		5.44		1.77	$\nu d_{3/2}^{-1} f_{7/2} (0.79)$
					· ·

One should contrast real phonons with pure p-h states.



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The Gamow-Teller resonance



$$\begin{array}{ll} \varepsilon_{\rm ph}^{(II)}, \varepsilon_{\rm ph}^{(I)} & {\rm Highe} \\ {\rm hole \ t} \\ \varepsilon_{\rm ph}^{(II)} - \varepsilon_{\rm ph}^{(I)} = \varepsilon_{j_{<}} \end{array}$$

Highest and lowest particlehole transitions in the picture

 $\varepsilon_{j>}$

Unperturbed GT energy related to the spinorbit splitting

$$\hbar\omega\approx\varepsilon_{\rm ph}+\langle V_{\rm res}\rangle$$

RPA GT energy related also to V in $\sigma\tau$ channel Osterfeld, 1992: Using empirical Woods-Saxon s.p. energies, the GT energy is claimed to determine g₀'

$$V_{\rm res} = g_0' \delta(\vec{r}_1 - \vec{r}_2) \sigma_1 \sigma_2 \tau_1 \tau_2$$

We want to go beyond the empirical description.



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