Nuclear single-particle and collective spectroscopy

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Fifth Gogny Conference Paris, 10th-13th Dec. 2024

Outline

• Quasi-particle states: particle-vibration coupling on top of EDFs

• The same model applied to collective states

• How to improve EDFs (short)

Single-particle states (I) all those is the set spectroscopic factor given below. Let us also below. Let us also be $d\mathbf{N}$ desirable since one expects that the residual that the residual the residual the residual the residual to \mathbf{N} \sim 111 states (or the three QP states) \mathcal{S} vibration coupling \mathcal{S} state energy of the odd nuclei which goes in the

mention that the proton density is distorted in-

Given an effective Hamiltonian H_{eff} , the single-particle (or quasi-particle) states can be calculated using HF (or HFB) $\frac{1}{2}$ are denight-hand side of $\frac{1}{2}$ m the basic quantities considered in all the studies considered in all the studies ϵ F (or HFR). The reason is that the F \mathbf{r} and \mathbf{r} <u>the original magnitude we need t</u> i quadi purticic, dialected

PHYSICAL REVIEW C VOLUME 21, NUMBER 4 APRIL 1980

the binding energies of the three adjacent nuclei.

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Hartree-Fock-Bogolyubov calculations with the $D1$ effective interaction on spherical nucle Hartree-Fock-Bogolyubov calculations with the $D1$ effective interaction on spherical h the $D1$ effective interaction on spherical $\mathbf r$

J. Dechargé and D. Gogny $\frac{1}{\sqrt{1-\frac{1$

Service de Physique Neutronique et Nucléaire, Centre d'Etudes de Bruyères-le-Châtel, Boîte Postale No. 561, A P R I L
 561, 92542 Montroug

No. 561, 92542 Montroug Cedex, France $(Received\ 3\ August\ 1979)$ la et Franceure, Centre a Braues de Brayeres-le-Chatel, Bone Fostale Fro. 501, 52542
Cedex, France $\text{N}\left(\text{N}\right)$ is a Highlian that $\text{N}\left(\text{N}\right)$ is a $\text{N}\left(\text{N}\right)$ is a set of only the e and D. Gogny
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Jex - Exance $\frac{1}{2}$ August $\frac{1}{2}$ and $\frac{1}{2}$

 $\frac{QF}{\text{vindition coupling}}$, would lower the ground
state energy of the odd nuclei which goes in the field in the framework of the Bogolyubov theory. First, a brief review of Hartree-Fock-Bogolyubov In Fig. 3 we have reported the HFB odd-even. mass differences along with the experimental studies on special reference to the pairing properties. In order to demonstrate the pairing properties. In order to demonstrate the pairing properties. values and we also give in Table V for each isotope the spin of its ground state as predicted in also tope the spin of its ground state as predicted by the HFB calculations. This we holice that
the HFB calculations reproduce the oscillating \blacksquare trends which are observed experimentally as a $\frac{1}{2}$ function of the noutron number. Concerning function of the neutron number. Concerning the above the experimental value by amount of the \int order of 200 koV. Somebow guch doviation is desirable since one expects that the residual \overrightarrow{id} interaction between the three QP states (or the
QP vibration coupling) would lower the ground
show that are some of the add unabiguities are in the state energy of the odd nuclei which goes in the right sense. Referring to the work of Kuo et $al.^{31}$. order of 300 keV. Somehow such deviation is $\begin{array}{|c|c|c|c|c|}\hline \end{array}$ $\begin{array}{|c|c|c|c|c|}\hline \end{array}$ would lower the ground Sh_0 \mathbf{Q} P vibration coupling) would lower the ground \mathbf{S} SNOU $\overline{}$ diagrams which are seen as players which are seen as posteriori to player to player $\overline{}$ by the HFB calculations. First we notice that magnitude of our predictions, they are all shifted above the experimental value by amount of the along with the experimental ions reproduce the oscillating

above the experimental value by an amount of the experimental value by an amount of the experimental value by order of 300 keV. Somehow such deviation is

Having no idea of the higherorder corrections we have no idea of which accuracy one should request

D1 and Dl'.

Single-particle states (II)

- We actually diagonalize H_{eff} in a basis made with 1p states plus 1p-1 phonon (RPA) states
- This has been generalised to 1 qp plus 1qp states-1 QRPA phonon states

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Skyrme EDFs (even-even nuclei)

They are **local** functionals depending on various densities.

Here, proton/neutron labels are omitted for the sake of simplicity.

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

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

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

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

$$
\vec{J}(\vec{r}) \text{ spin}-\text{orbit density}
$$

 $C^{\rho\rho}[\rho] = A + B\rho^{\gamma}$

fit to data (or pseudo-data). $\begin{bmatrix} 5 \end{bmatrix}$ Parameters are determined by a

(Quasi)particle-vibration coupling (I)

• The model is self-consistent (no empirical input). We employ H_{Skyrme} but one can think of using it with any Hamiltonian

$$
H = H_0 + V,
$$

\n
$$
H_0 = \sum_{jm} \varepsilon_j a_{jm}^{\dagger} a_{jm} + \sum_{NJM} \hbar \omega_{NJ} \Gamma_{NJM}^{\dagger} \Gamma_{NJM},
$$

\n
$$
V = \sum_{jmj'm'} \sum_{NJM} \frac{\langle j||V||j', NJ\rangle}{\hat{j}} a_{jm} \left[a_{j'}^{\dagger} \otimes \Gamma_{NJ}^{\dagger} \right]_{jm},
$$

• We correct for the non-orthonormality and overcompleteness of the basis by introducing the NORM matrix

$$
n(j'_1n_1J_1,j'_2n_2J_2) = \delta(j'_1,j'_2)\delta(n_1,n_2)\delta(J_1,J_2) - \sum_{h_1}(-)^{J_1+J_2+j'_1+j'_2}j_1j_2\left\{\begin{array}{ccc}j'_2 & j_{h_1} & J_1 \\ j'_1 & j & J_2\end{array}\right\}X_{j'_2h_1}^{(n_1J_1)}X_{j'_1h_1}^{(n_2J_2)}
$$

$$
\overline{(\mathcal{H}-\mathcal{N}E)\,\Psi=0}
$$

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49

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stituto Nazionale di Fisica Nuclear

Energies and γ **transitions in Ref. [5] are shown as Spectroscopic factors of ⁴⁹Ca**

Results obtained with SkX γ -ray branching ratios and intensities were reported and a correlations, engineering us to extract multiplomation with the mixing us to extract multiplomation and mixing the mixing of the mixing of

^aThe authors report the errors on C²S for the $5/2^-$ and $9/2^+$ states as "a few percent". observed, although the HCM model between \mathbf{r}

TABLE X. Experimental and theoretical (see [8] and references therein) C^2S spectroscopic factors for the $9/2^+$ at 4296 keV in ⁴⁹Ca.

Experiment	C^2S
(d, p) [72] 12 C + 48 Ca [8]	0.14 0.27(1)
Theory	C^2S
HCM	0.11
GXPF1 [8]	0.42

S. Bottoni et al., Phys. Rev. C103, 014320 (2021) $\hskip1cm \overline{7}$

quenching of spectroscopic factor for the 9*/*2⁺ state in 49Ca,

The subtraction scheme

$$
\Sigma(E) \rightarrow \Sigma(E) - \Sigma(E = 0)
$$

- This prescription has been introduced in the context of the theories beyond RPA for the collective excitations, when based on EDFs
- The goal is to avoid the double-counting of static correlations
- It also avoids undesired divergences ("renormalization")
- It can be implemented with the same aim(s) when considering single-particle spectroscopy
- Note: working with pairing sets a zero-energy for quasi-particles

IS689: Single-particle structure along N=127: ²¹²Rn(d,p)²¹³Rn

VERY PRELIMINARY RESULTS courtesy of D. Clarke, D.K. Sharp (University of Manchester)

Comparison with DFT+QPVC

Note: theory reports the absolute S_F , while in experiment the values are normalized to the g.s. S_F

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Random Phase Approximation

$$
h\phi_i=\varepsilon_i\phi_i
$$

In the time-dependent case, one can solve the evolution equation for the density directly:

$$
h(t) = h + f(t) \qquad [h(t), \rho(t)] = i\hbar \dot{\rho}(t)
$$

$$
\rho(t=0) \neq \rho_{\rm g.s.}
$$

$$
\rho(t = \Delta t) = U(t = 0, t = \Delta t)\rho(t = 0) \qquad U = e^{-i\frac{\Delta t}{\hbar}}
$$

If the equation for the density is linearized and solved on a basis: **Random Phase Approximation or RPA**.

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

 $\frac{1}{10}$ The Governoe control on $\frac{1}{10}$ december 2024 11 In RPA the excited states are 1p-1h superpositions

From: P. Stevenson (U. Surrey)

$$
U = e^{-i\frac{\Delta t}{\hbar} \cdot h}
$$

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

(Q)RPA + (Q)PVC

 $\left(A + \Sigma(E) \quad B\right)$ $-B$ $-A - \Sigma^*(-E)$

The state α is 1p-1h plus one phonon.

The scheme is very effective to produce GR widths. It also produces a downward shift of the GRs.

$$
\Sigma(E) \approx \int dE' \frac{V^2}{E - E' + i\epsilon}
$$

$$
\frac{1}{E - E' + i\epsilon} \rightarrow \frac{1}{E - E'} - i\pi \delta(E - E')
$$

FIFTH GOGING FOR ALCOHOL WE HAVE A SCHEME INCLUDING

Nuclear incompressibility and the ISGMR

Isoscalar Giant Monopole Resonance or "breathing mode": its energy should be correlated with the incompressibility of nuclear matter.

$$
K_{\infty} = 9\rho_0^2 \frac{d^2}{d\rho^2} \left(\frac{E}{A}\right)_{\rho=\rho_0}
$$

$$
\chi \equiv -\frac{1}{\Omega} \left(\frac{\partial P}{\partial \Omega} \right)^{-1}
$$

$$
\chi^{-1} = \rho^3 \frac{d^2}{d\rho^2} \left(\frac{E}{A}\right)
$$

Impact on astrophysics: supernova explosion, neutron star merging

PHYSICAL REVIEW LETTERS 129, 032701 (2022)

Probing the Incompressibility of Nuclear Matter at Ultrahigh Density through the Prompt Collapse of Asymmetric Neutron Star Binaries

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Fifth Gogny conference, 10-13 December 2024 Fifth Gogny conference, 10-13 December 202 Department of Physics, Pennsylvania State University, University Park, Pennsylvania 16802, USA ⁷

How correlated are E_{ISGMR} and K_{∞} ?

Only self-consistent DFT calculations that treat **uniform matter and the response of finite nuclei on equal footing** allow extracting K_∞

J.P. Blaizot, Phys. Rep. 64, 171 (1980)

There are different sources of model dependence in this procedure.

One **key point** is that different EDFs have different assumptions for the density dependence.

GC *et al.*, Phys. Rev. C70 (2004) 024307.

• Sensitivity to the choice of the nucleus?? $\frac{1}{14}$

From the ISGMR measured in 208Pb one extracts:

 $K_{\infty} = 240 \pm 20$ MeV

U. Garg, GC, PPNP 101 (2018) 55

However, in even-even ¹¹²⁻¹²⁴Sn, the ISGMR centroid energy is overestimated by about 1 MeV by the same models, which reproduce the ISGMR energy well in 208Pb. **Fig. 10.** (Color online) RPA calculations of the monopole strength in 208Pb, performed by using the nonrelativistic Skyrme-type functional SAMi [42], the \mathbf{u} , \mathbf{u}

Why is Tin so soft?

Pairing can partly explain the problem but with some remaining ambiguity.

i Fisica Nuclear

In our work, we have been able, for the first time, to analyse **in a systematic manner** the consistency between ISGMR energies in different nuclei.

We have used many Skyrme EDFs.

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

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

Fig. 2023 Rev. Lett. 131, 082501 (2023) Z.Z. Li, Y.F. Niu, GC, Phys.

ISGMR in Sn isotopes

- Exp. data from D. Patel *et al*., Phys. Lett. B726, 178 (2013)
- QPVC reproduces the experimental data quite well.
- The best description is obtained with the Skyrme EDF SV-K226.

Klüpfel, Reinhard, *et al.*, PRC 79, 034310 (2009)

Other applications of QPVC

present work compared with QRPA calculations including \mathbb{Z}

normalized to each other at 20 MeV. The 20

 $\mathcal{L}_{\mathcal{A}}$ from the spectrum at a scattering angle of 0*.*40[→] using the virtual photon method (blue circles). a \mathcal{R} and \mathcal{R} Comparison with very recent data from (p,p') measured at RCNP, Osaka.

Exp. data from I. Brandherm *et al.*

Theory reproduces very well the dipole polarizabilty and can be used to estimate the high-energy dipole tail.

| arXiv:2410.00610v1 [nucl-ex] 1 Oct 2024

• Quasi-particle states: particle-vibration coupling on top of EDFs

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Bayesian inference of a Skyrme EDF

- **TABLE III. Means in the marginalized posterior deviations of the marginalized posterior deviations in the seven in** • Results are in line with other types of analysis, except for a tendency
	- Tension associated with A_{PV}(²⁰⁸Pb) *RA R*_c_{*C*} *<i>R_c*^{*R*} *<i>R_c*^{*C*} *<i>C <i>C <i>C <i>C <i>C C C C <i>C C C C C C C C C C C C*
	- Fifth Gogny conference, 10-13 December 2024 20 ε0 *µ* 0*.*162 0*.*161 0*.*160 0*.*161 0*.*161 0*.*162 0*.*161 ϑ 0*.*005 0*.*005 0*.*004 0*.*004 0*.*004 0*.*004 0*.*004 • Still not possible at the level beyond EDF (e.g. including QPVC)

µ →15*.*96 →15*.*97 →15*.*93 →15*.*93 →15*.*91 →15*.*96 →15*.*94

FIG. 2. Marginalized posterior distributions of parameters for the seven inferences.

Ab initio-based EDFs *Nuclear Density Functional Theory (DFT): perspectives and* ab initio*-based functionals* Gianluca Colò

Conclusions

- Not only DFT is the only theory for heavy nuclei, but also the only theory for highly excited states
- The dynamical correlations associated with the **quasiparticle-vibration coupling (QPVC) approach** have been introduced on top of DFT and shown to be essential for solving the problem of the nuclear incompressibility
- Our method also allows studying the fragmentation of the single-particle strength and its evolution
- We are currently working on new EDFs, either based on *ab initio* or on Bayesian inference from experimental data

- C. Barbieri, E.Vigezzi (Univ. of Milano and INFN, Italy)
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- P. Klausner, M. Antonelli, F. Gulminelli (LPC Caen, France)
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• Z.Z. Li, Y. Niu (Lanzhou University)

[https://ns4exp.mi.inf](https://ns4exp.mi.infn.it/)n.it

The Structure4exp virtual access (VA) facility, at ns4exp, mi, infn, it, is a part of the Theo4Exp VA infrastructure and, as such, is intended to provide theoretical tools for the EURO-LABS project as well as for the wider nuclear physics community. The key nuclear structure codes available are now either HF plus RPA and HFBCS plus ORPA for spherical nuclei, or a shell model code. All, in different ways, produce output for basic observable quantities that are the subject of current experimental activity:

- i. Binding energies, density distributions and mean square radii
- ii. Energies and wave functions/transition densities of the excited states
- iii. Electromagnetic transition probabilities to the ground state.

This facility includes three codes:

Random Phase Approximation (RPA) plus Hartree Fock (HF) HF Bardeen Cooper Schrieffer-Quasiparticle RPA (HFBCS-QRPA) **KSHELL** code

Backup slides

Fifth Gogny conference, 10-13 December 2024 25

The Kohn-Sham scheme

We assume that the density can be expressed in terms of **single-particle orbitals**, and that the kinetic energy has the simple form:

$$
\rho(\vec{r}) = \sum_{i} \phi_i^*(\vec{r}) \phi_i(\vec{r}) \qquad T = \sum_{i} \int d^3r \; \phi_i^*(\vec{r}) \left(-\frac{\hbar^2 \nabla_i^2}{2m} \right) \phi_i(\vec{r})
$$

We have said that the energy must be minimized, but we add a constraint associated with the fact that we want **orbitals that form an orthonormal set** (Lagrange multiplier):

$$
E - \sum_{i} \varepsilon_{i} \int d^{3}r \; \phi_{i}^{*}(\vec{r}) \phi_{i}(\vec{r}) = T + F[\rho] + \int d^{3}r \; V_{\text{ext}}(\vec{r}) \rho(\vec{r}) - \sum_{i} \varepsilon_{i} \int d^{3}r \; \phi_{i}^{*}(\vec{r}) \phi_{i}(\vec{r})
$$

The variation of this quantity, $(\delta/\delta\phi^*)$... = 0 produces a Schrödinger-like equation:

$$
\left(-\frac{\hbar^2 \nabla_i^2}{2m} + \frac{\delta F}{\delta \rho} + V_{\text{ext}}\right) \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r}) \quad h \phi_i = \varepsilon_i \phi_i
$$

"DFT is an exactification of Hartree-Fock" (W. Kohn).

Simple interpretation

• RPA or QRPA based on EDFs includes only 1p-1h excitations.

(GC *et al*., Comp. Phys. Comm. 184, 142, 2013; N. Paar *et al*., Rep. Prog. Phys. 70, 691, 2007)

• One would like to aim at calculations in which many nucleons are excited. But SM calculations can be performed only in light nuclei.

(S.E. Koonin *et al*., Phys. Rep. 278, 1, 1997; E. Caurier *et al*., Rev. Mod. Phys. 77, 427, 2005)

• QPVC stays somehow in between. 2p-2h excitations are included, and the ring diagrams are summed in the intermediate states.

Some detail + the subtraction scheme

All QRPA calculations are performed in a model space which is large enough so that the EWSR is satisfied.

We calculate natural-parity phonons with 0^+ , 1⁻, 2^+ ... 5⁻ and select those having energy less than 30 MeV and strength larger than 2% of the total strength.

The convergence of the results with respect to the choice of the model space has been carefully assessed.

$$
\Sigma(E)
$$

$$
\text{Subtraction:}\qquad \Sigma(E)\quad\rightarrow\quad \Sigma(E)-\Sigma(E=0)
$$

- \blacksquare Fig. 1. (Coloring functions in the strength functions in even-even-even-even-even-even-either \blacksquare L_{ν} , data hom in Lorentzian having a width of 1 MeV (2007) and 0.D. Olorunfunmi, Phys. Rev. C 105, 054319 (2022). • Exp. data from T. Li *et al*., Phys. Rev. Lett. 99, 162503 (2007) and S.D.
	- In these two cases there is no pairing.

The energy shift from QRPA to QPVC

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

$$
\Delta E_c = E_c(\text{QRPA}) - E_c(\text{QPVC})
$$

 $E_c = \sqrt{m_1/m_{-1}}$

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

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

The mechanism behind the energy shift

$$
\Sigma(E) \approx \int dE' \frac{V^2}{E - E' + i\epsilon}
$$

$$
\frac{1}{E - E' + i\epsilon} \to \frac{1}{E - E'} - i\pi \delta(E - E')
$$

The **real part of the self-energy** produces the energy shift

E = **QPVC** energy of the GMR E' = energy of the **doorway states** 2 q.p. \otimes 1 phonon

re two nuclei, but doorway state energies The QPVC energy is not very different in the two nuclei, but doorway state energies are higher in Sn than in Pb

The pairing gap Δ makes the relative energy position of the ISGMR and of the doorway states different!

| More applications of QPVC: β-decay **TREE INTERACTER INTERS** IN THE **INTER** The resulting calculated lifetimes for the results for the set σ are compared with the RPA results in Fig. 3. The RPA results agencies marked in the half-lives for all the half-lives for all \sim nuclei. An exception is represented by the interaction is represented by the interaction is represented by the to perform well in magic nuclei as far as the line shape of s ot WPVC: B-decay $\overline{}$

182 the proton-neutron pairing, and in particular its isoscalar *T* = 0 component, is still elusive [cf. (Sagawa

this peak contributes 22% of the total 1=T1=2.

 $V \Gamma$ Nin at all Dhim Day half-114 (140E01 \overline{M} Y. F. Niu *et al.*, Phys. Rev. Lett. 114, 142501 **In** Figure 3. -decay half-lives in the case of 132Sn, 68Ni, 34Si, and 78Ni, 34Si, and RPA and RPA

lar, the interaction SkM* that had been previously shown

we can expect that including the effect of PVC will also expect of PVC will also expect of PVC will also expect

 $\begin{bmatrix} 10^3 \end{bmatrix}$ $\begin{bmatrix} 1 & 1 \ 1 & 1 \end{bmatrix}$ SLys $\begin{bmatrix} 1 & 1 \ 1 & 1 \end{bmatrix}$ a main peak, it does note ontoriant. ount for sprea 0 OPVC remedia $\left[\begin{array}{c} \begin{array}{c} \text{10}^{\circ} \\ \text{10}^{\circ} \end{array} \right] \qquad \begin{array}{c} \text{11}^{\circ} \\ \text{22}^{\circ} \end{array} \right] \qquad \text{strength. QPVC remedies to this shortcoming.}$ $\begin{bmatrix} \hat{x} & 10^2 \\ \hat{y} & \hat{z} & \hat{z} \end{bmatrix}$ and $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ and frequential proton \hat{z} inspired by Figure is i 8 of (Rubio et al. (2020)). (Right panel) Schematic view of the different approximations to calculate the not account for spread and fragmentation of the While QRPA collects the simple two-

particle and Astrophysics (Adam Hilger, Bristol, 1990). c case or p-uecay, and is p important because of the phase-space factor. "Sn"Ni "Si"Ni "Sn"Ni "Si"Ni likelihood of β-decay, this is particularly

Nuclei are finite systems and the dependence of the EDF on ∇_{ρ} , τ and *J* is mandatory. These quantities vanish in uniform matter.

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

Uniform matter perturbed by a (weak) periodic potential

