Nuclear Energy Density Functionals and Collective Excitations

Dario Vretenar
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Exotic Modes of Excitation Far From Stability

Characteristic ground-state properties (weak binding of the outermost nucleons, coupling between bound states and the particle continuum, nuclei with very diffuse neutron densities, formation of neutron skin and halo structures) have a pronounced effect on the multipole response of unstable nuclei.

The enhancement of the low-lying multipole strength is a general phenomenon in systems characterized by small values of particle (e.g. neutrons) separation energies.

IOP PUBLISHING REPORTS ON PROGRESS IN PHYSICS

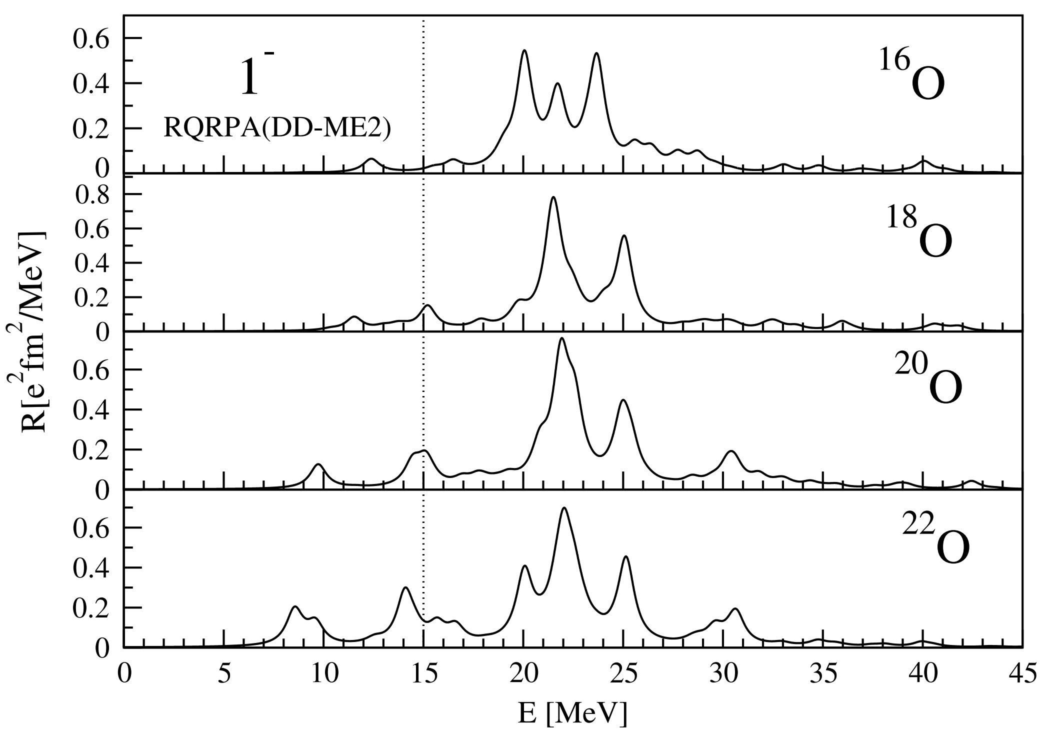
Rep. Prog. Phys. **70** (2007) 691–793 doi:10.1088/0034-4885/70/5/R02

Exotic modes of excitation in atomic nuclei far from stability

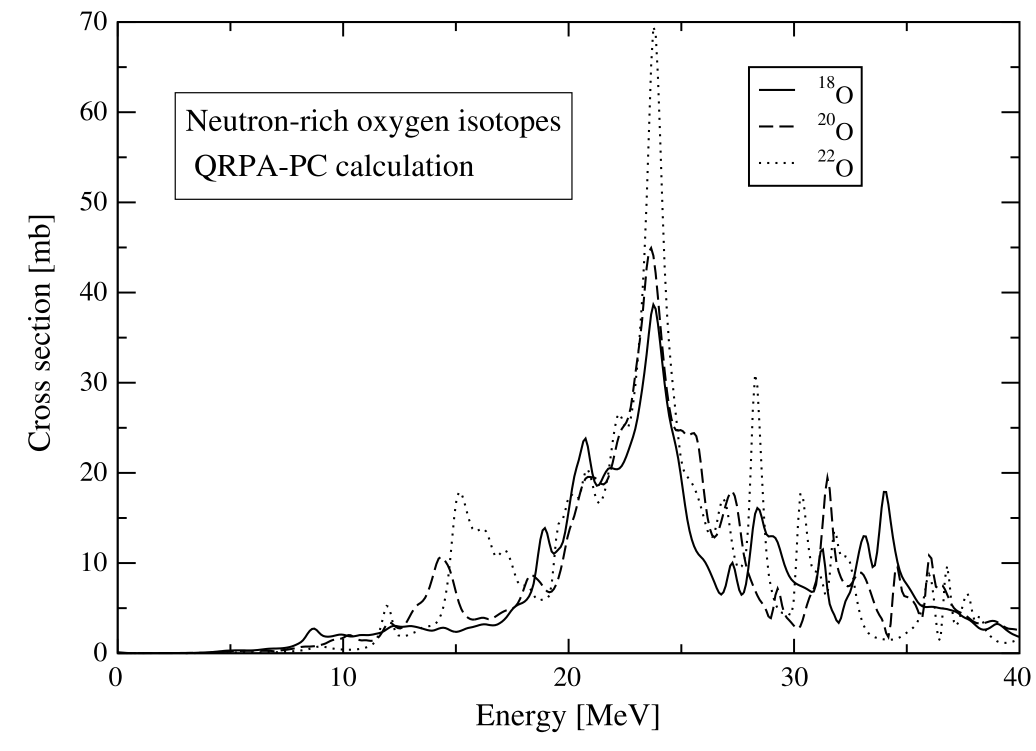
Nils Paar[1,2], Dario Vretenar[2], Elias Khan[3] and Gianluca Colò[4]

Low-energy electric dipole strength

Isovector dipole strength → RHB + RQRPA.



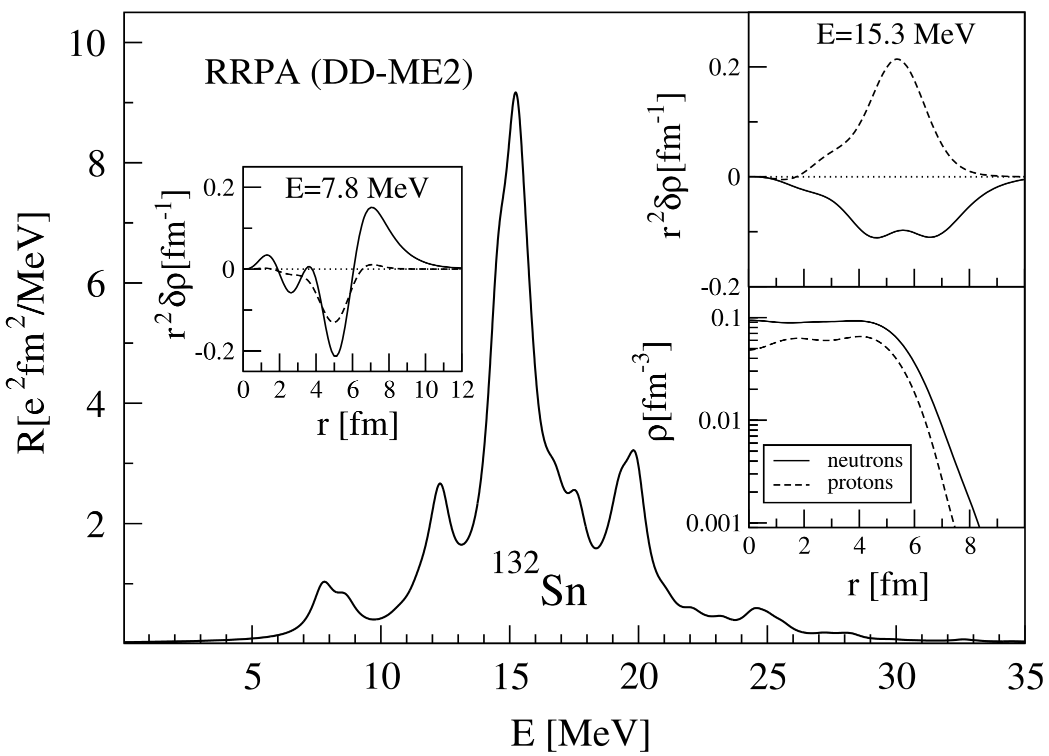
QRPA plus phonon coupling.

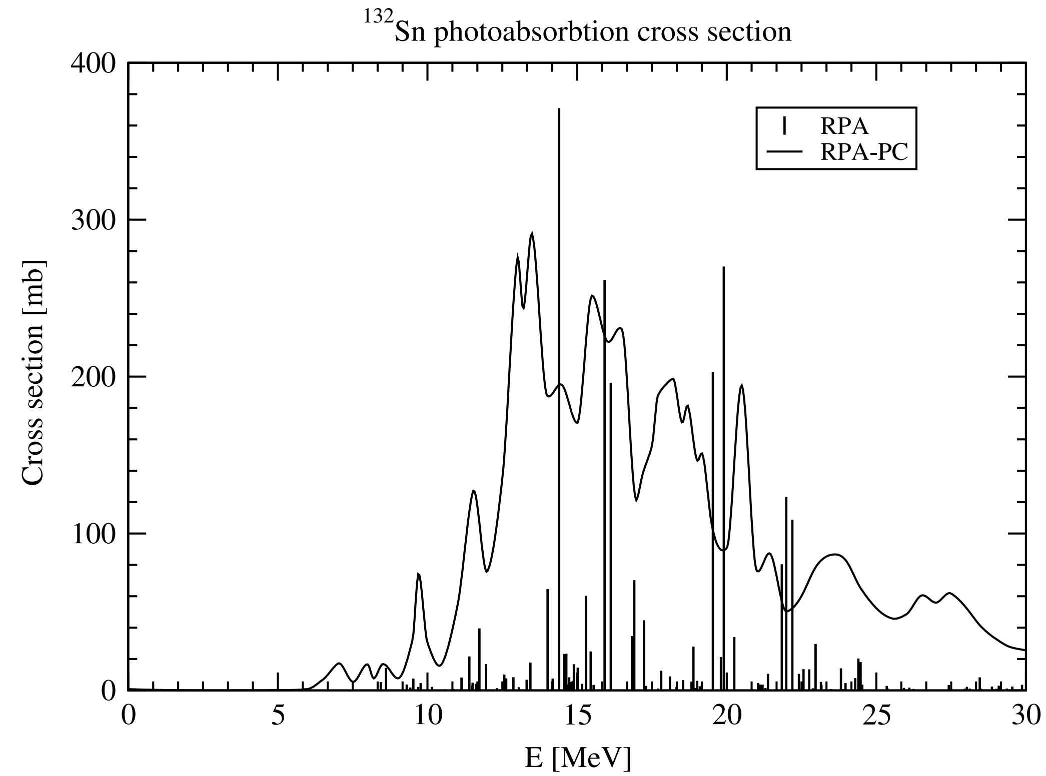


All models agree on the overall effect of the neutron excess on the E1 transition strength. The inclusion of particle–vibration coupling brings the results in closer agreement with experiment.

… dipole strength in the low-energy region is caused by non-resonant single-particle excitations of the last bound neutrons.

Pygmy dipole resonances in heavier neutron-rich nuclei





A single collective dipole state below 10 MeV. Its RRPA amplitude presents a coherent superposition of neutron p–h configurations.

RPA-PC → none of the peaks below 10 MeV contain contributions of more than two or three different neutron particle–hole (ph) configurations.

The inclusion of particle–vibration coupling in (Q)RPA improves the agreement between the calculated and empirical widths of the GDR structures, and also has a pronounced effect on the low-lying E1 strength.

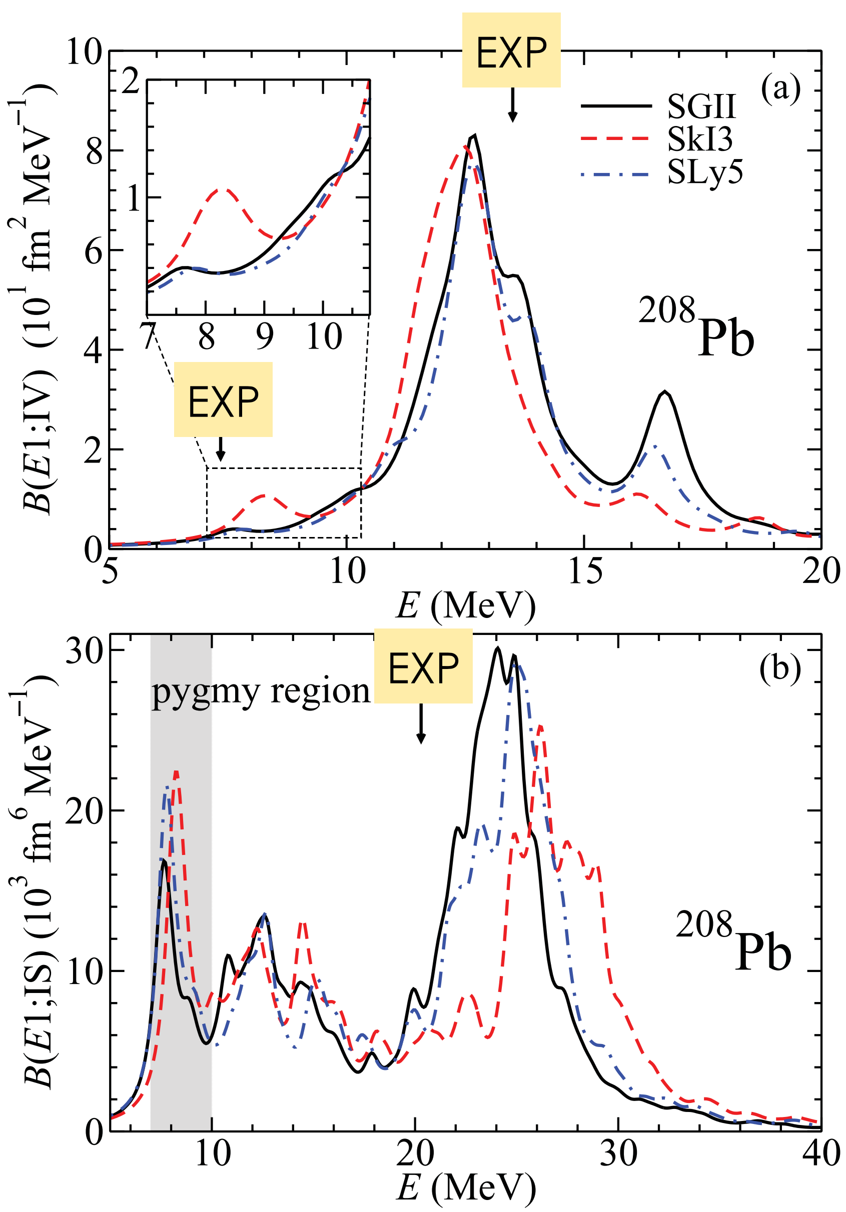
Collectivity and Isospin Character of Pygmy Dipole Strength?

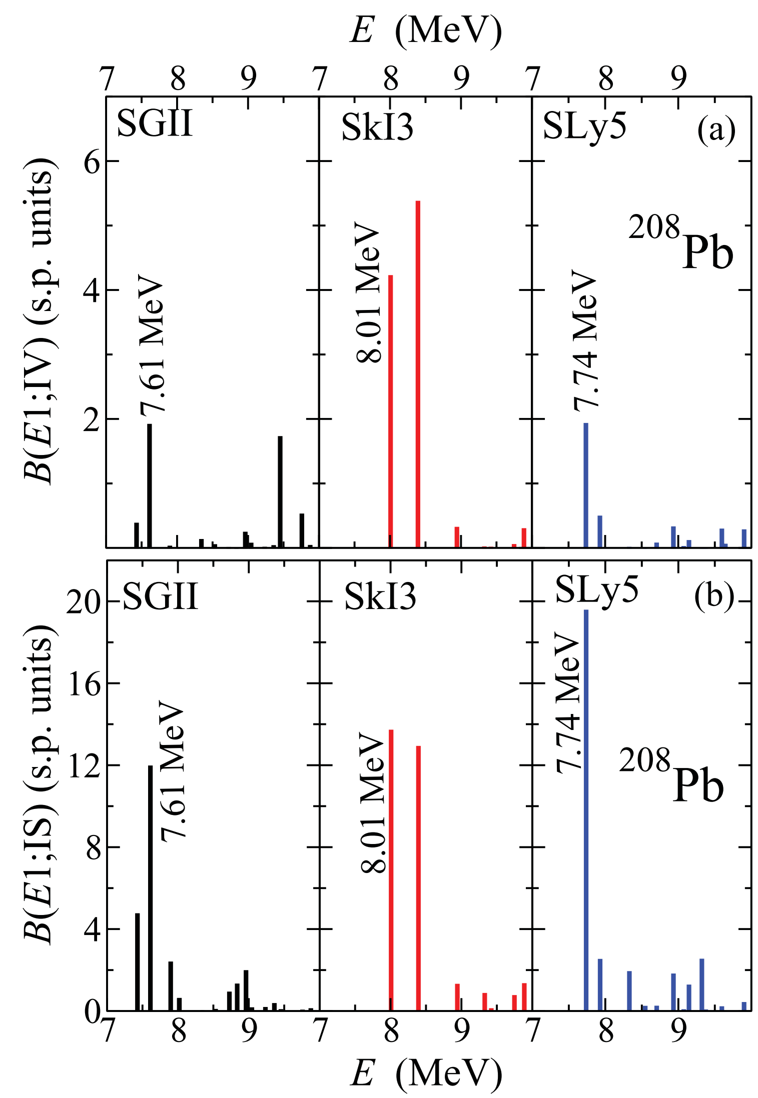
LANZA, CATARA, GAMBACURTA, ANDRÉS, AND CHOMAZ — PHYSICAL REVIEW C **79**, 054615 (2009)

D. VRETENAR, Y. F. NIU, N. PAAR, AND J. MENG — PHYSICAL REVIEW C **85**, 044317 (2012)

ROCA-MAZA, POZZI, BRENNA, MIZUYAMA, AND COLÒ — PHYSICAL REVIEW C **85**, 024601 (2012)

RPA strength functions for the isovector and isoscalar dipole response



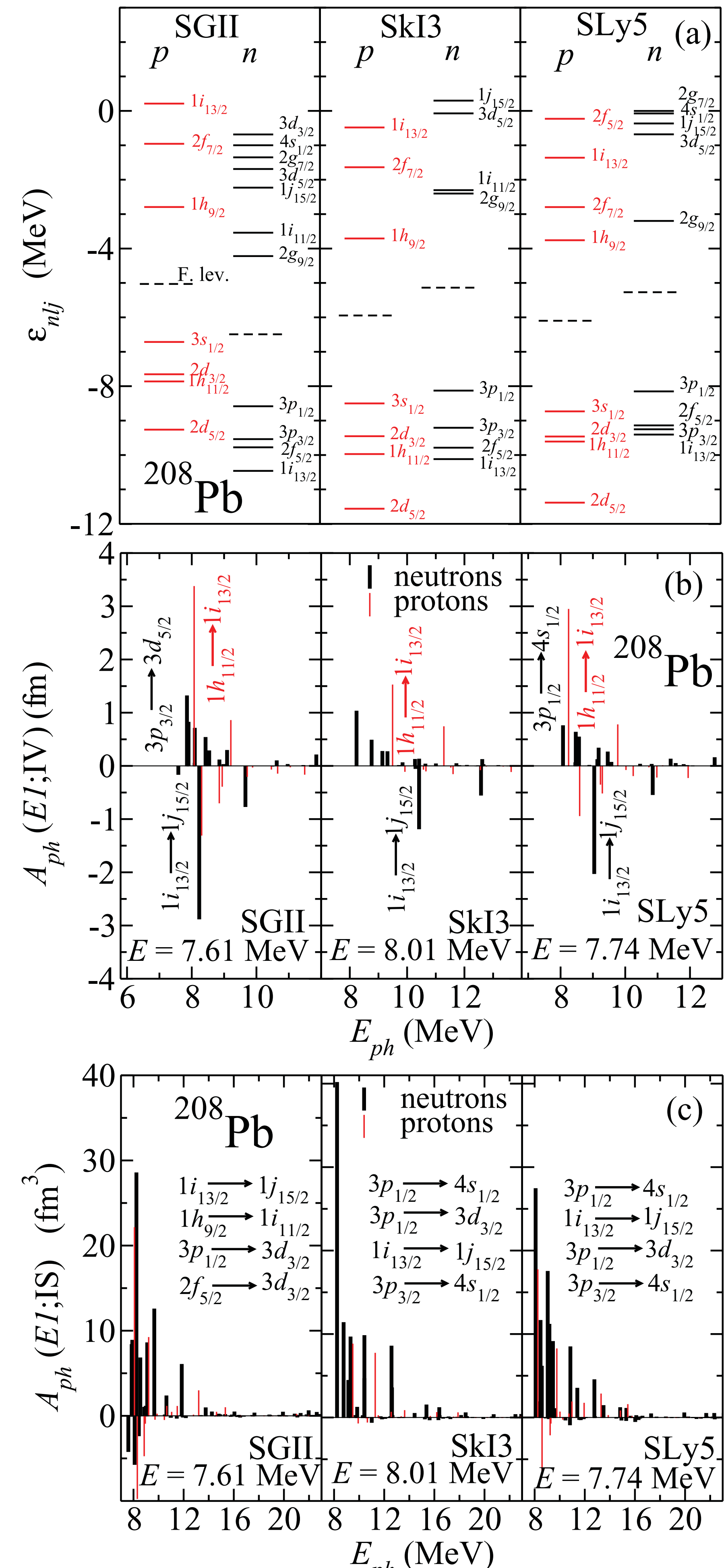


Reduced transition probabilities

Reduced transition probabilities

$$B(EJ,\tilde{0}\rightarrow\nu) = |\langle\nu||\hat{F}_J||\tilde{0}\rangle|^2$$
$$= \left|\sum_{\rm ph}\left(X^{(\nu)}_{\rm ph}+Y^{(\nu)}_{\rm ph}\right)\langle p||\hat{F}_J||h\rangle\right|^2,$$

… reduced amplitude: $A_{\rm ph}(EJ,\tilde{0}\rightarrow\nu) = \left(X^{(\nu)}_{\rm ph}+Y^{(\nu)}_{\rm ph}\right)\langle p||\hat{F}_J||h\rangle.$



Isovector reduced amplitude of the PDS → destructive interference of a small number of particle-hole configurations. The reduced transition probability does not exceed ≈ 2-4 single-particle units.

Isoscalar channel → coherent superposition of neutron particle-hole configurations. Collective response of the PDS to the isoscalar dipole operator ≈10 - 20 single-particle units.

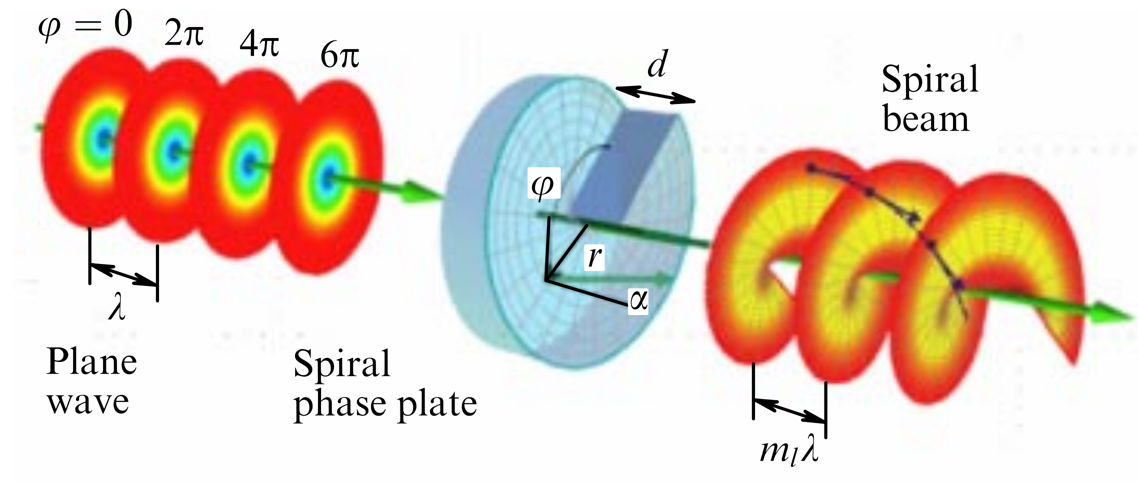
Nuclear Science and Techniques (2023) 34:189
https://doi.org/10.1007/s41365-023-01343-8

RESEARCH HIGHLIGHT

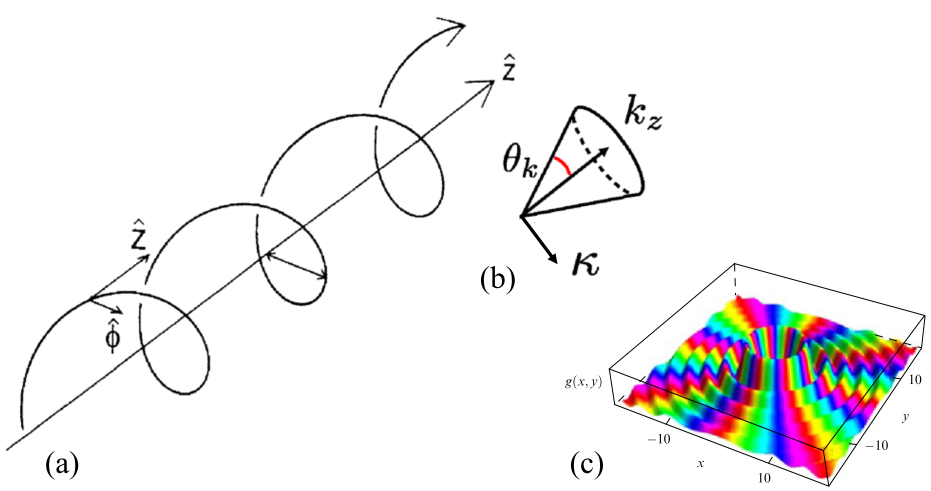
Vortex photons

A novel way to study the nuclear collective excitations

Gianluca Colò[1,2]



Twisted (vortex) states: solutions of the wave equation in cylindrical coordinates



$$\psi_{\varkappa m k_z}(\mathbf{r}) = J_m(\varkappa\rho)\exp\left[\mathrm{i}(m\varphi_r + k_z z)\right].$$

They differ from plane waves by the existence of a nonzero projection of the orbital angular momentum on the direction of propagation, and from spherical waves by the existence of a certain direction of propagation.

The projection m of the orbital angular momentum is a good quantum number for twisted states, while the values of the angular momentum: $l \geq |m|$.

Selective excitations of resonances

Manipulation of Giant Multipole Resonances via Vortex γ Photons

Zhi-Wei Lu, Liang Guo, Zheng-Zheng Li, Mamutjan Ababekri, Fang-Qi Chen, Changbo Fu, Chong Lv, Ruirui Xu, Xiangjin Kong, Yi-Fei Niu, and Jian-Xing Li

Phys. Rev. Lett. **131**, 202502

Giant resonances with specific multipolarity can be selectively excited by vortex photons.

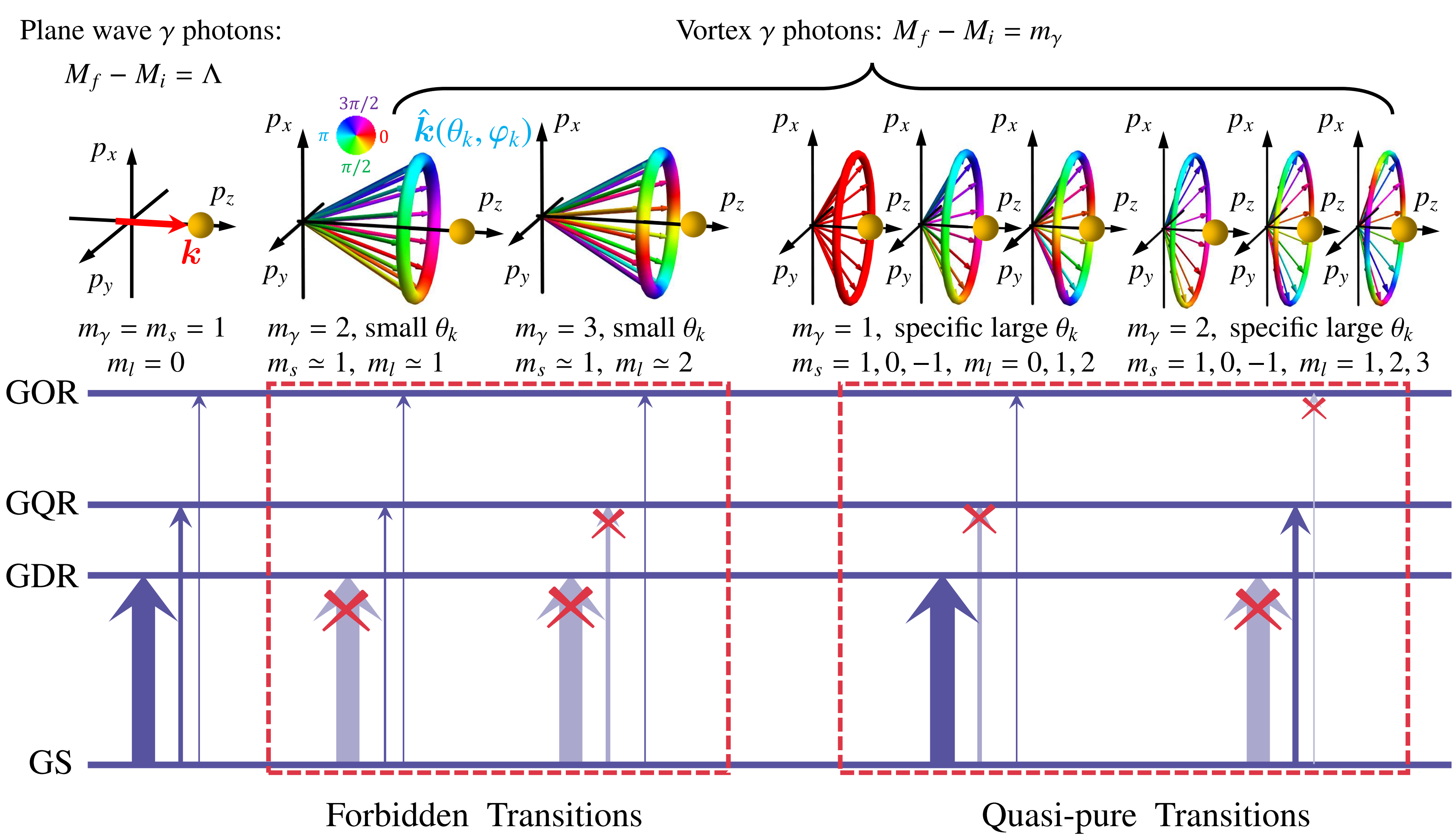
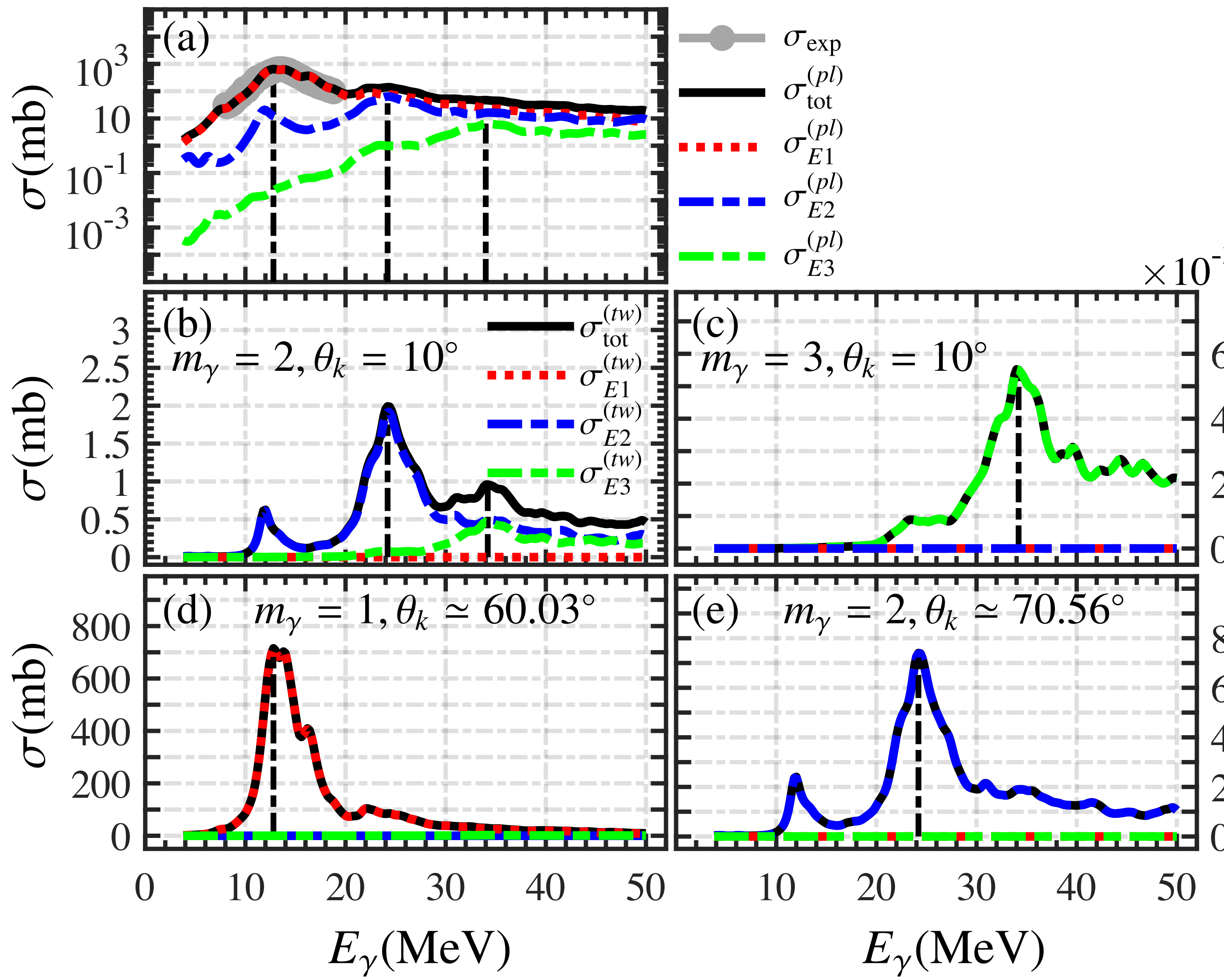


Photo-absorption cross sections for ^{208}Pb.

Plane waves ($m_l = 0$)

Vortex photons ($m_l \neq 0$)



Symmetry Energy

… energy per particle in nuclear matter: $$\frac{E}{A}(\rho,\beta) = \frac{E}{A}(\rho,\beta=0) + S(\rho)\beta^2. \qquad \beta \equiv (\rho_n - \rho_p)/\rho$$

Symmetry energy: difference between the energy per particle E/A in pure neutron and symmetric matter.

$$S(\rho) = J + L\left(\frac{\rho-\rho_0}{3\rho_0}\right) + \frac{1}{2}K_{sym}\left(\frac{\rho-\rho_0}{3\rho_0}\right)^2 + \ldots,$$

$$J \equiv S(\rho_0),\ L \equiv 3\rho_0\ S'(\rho_0),\ \text{and}\ K_{\rm sym} \equiv 9\rho_0^2\ S''(\rho_0).$$

… what is the density dependence of the symmetry energy?

Which nuclear properties are most sensitive to the symmetry energy?

Excitation energy of GDR, pygmy E1, IV GQR, neutron skin thickness…

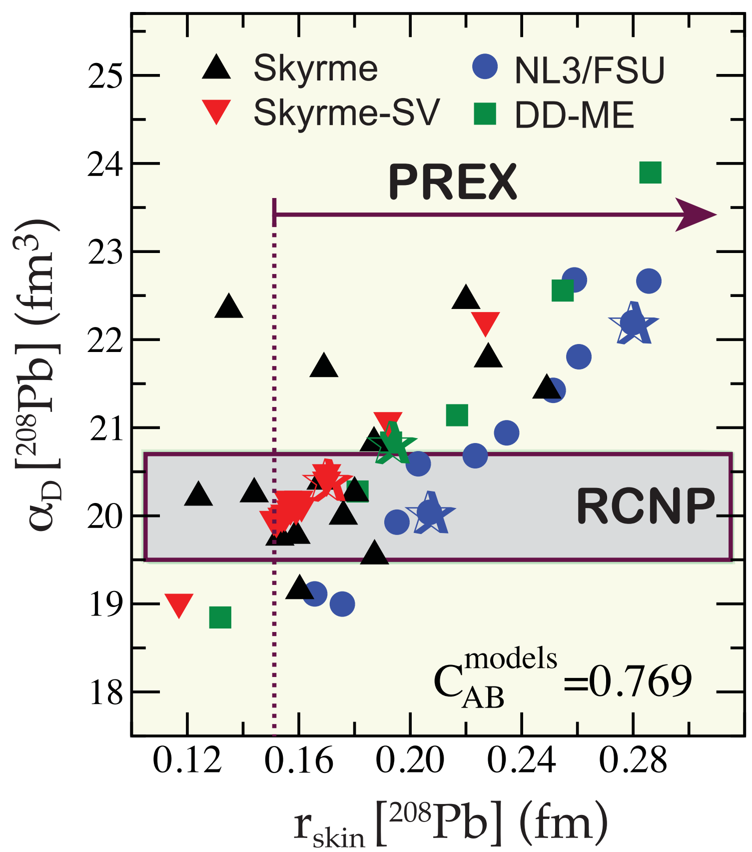
PHYSICAL REVIEW C **85**, 041302(R) (2012)

Electric dipole polarizability and the neutron skin

J. Piekarewicz,[1] B. K. Agrawal,[2] G. Colò,[3,4] W. Nazarewicz,[5,6,7] N. Paar,[8] P.-G. Reinhard,[9] X. Roca-Maza,[4] and D. Vretenar[8]

GDR → for this isovector mode the symmetry energy provides the restoring force. The dipole polarizability:

$$\boxed{\alpha_D = \frac{8\pi e^2}{9}\int_0^\infty \omega^{-1} R(\omega; E1)\, d\omega = \frac{8\pi e^2}{9} m_{-1}(E1),}$$



Measured value of the E1 polarizability ⇒ constraint on the neutron-skin thickness of ^{208}Pb.

PHYSICAL REVIEW C **87**, 034301 (2013)

Giant quadrupole resonances in ^{208}Pb, the nuclear symmetry energy, and the neutron skin thickness

PHYSICAL REVIEW C **88**, 024316 (2013)

Electric dipole polarizability in ^{208}Pb: Insights from the droplet model

PHYSICAL REVIEW C **92**, 064304 (2015)

Neutron skin thickness from the measured electric dipole polarizability in ^{68}Ni, ^{120}Sn, and ^{208}Pb

PHYSICAL REVIEW LETTERS **120**, 202501 (2018)

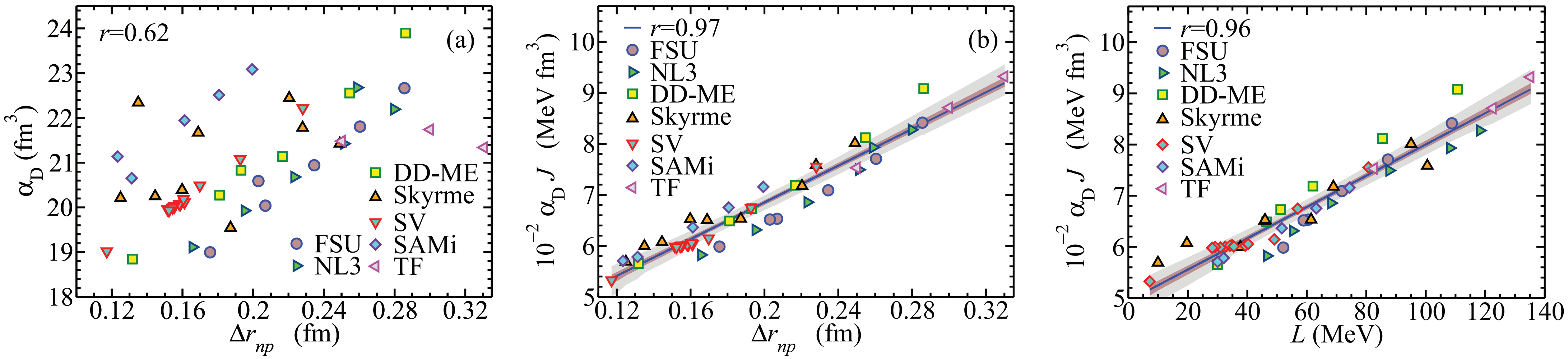
Nuclear Symmetry Energy and the Breaking of the Isospin Symmetry: How Do They Reconcile with Each Other?

Progress in Particle and Nuclear Physics 101 (2018) 96–176

Nuclear equation of state from ground and collective excited state properties of nuclei

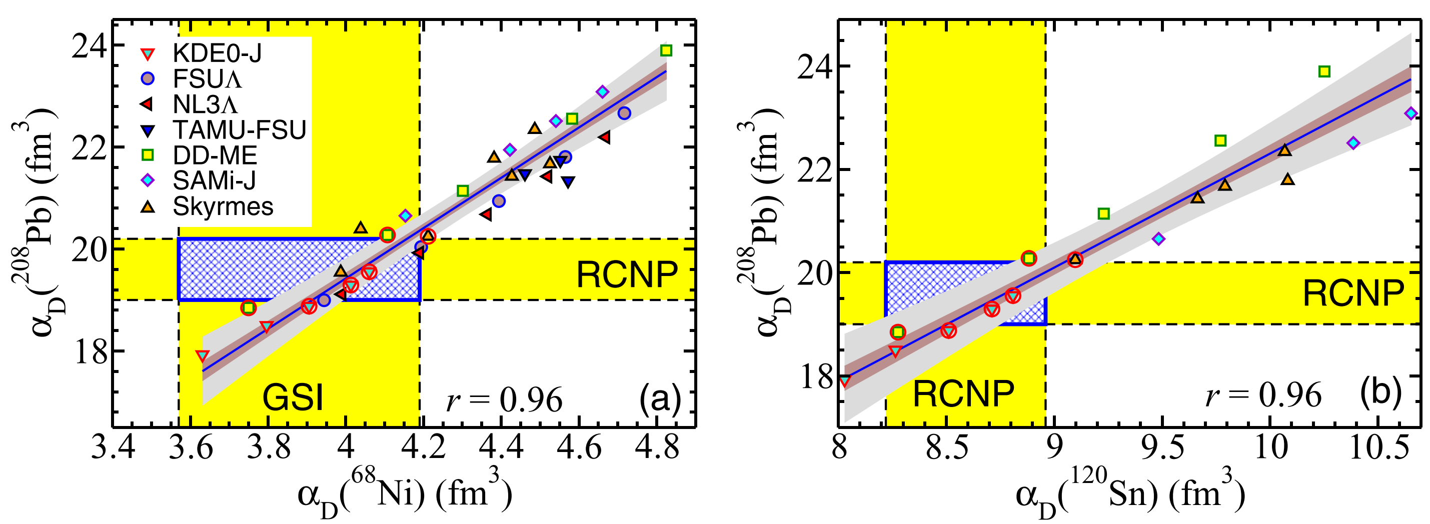
Dipole polarizability vs neutron skin thickness of ^{208}Pb

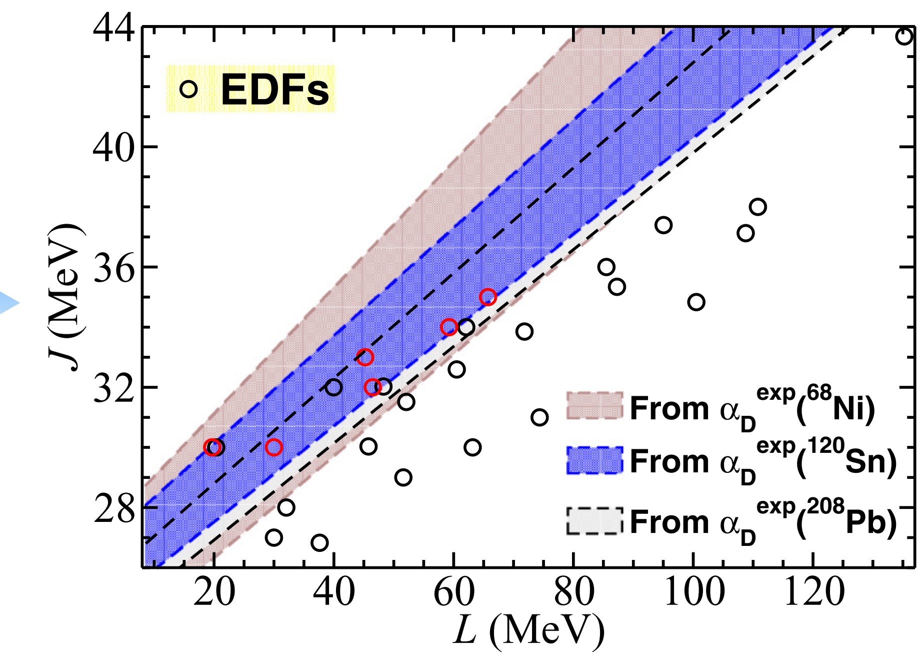
X. ROCA-MAZA *et al.* PHYSICAL REVIEW C **88**, 024316 (2013)



Neutron skin thickness from the measured electric dipole polarizability of ^{68}Ni, ^{120}Sn, and ^{208}Pb

PHYSICAL REVIEW C **92**, 064304 (2015)



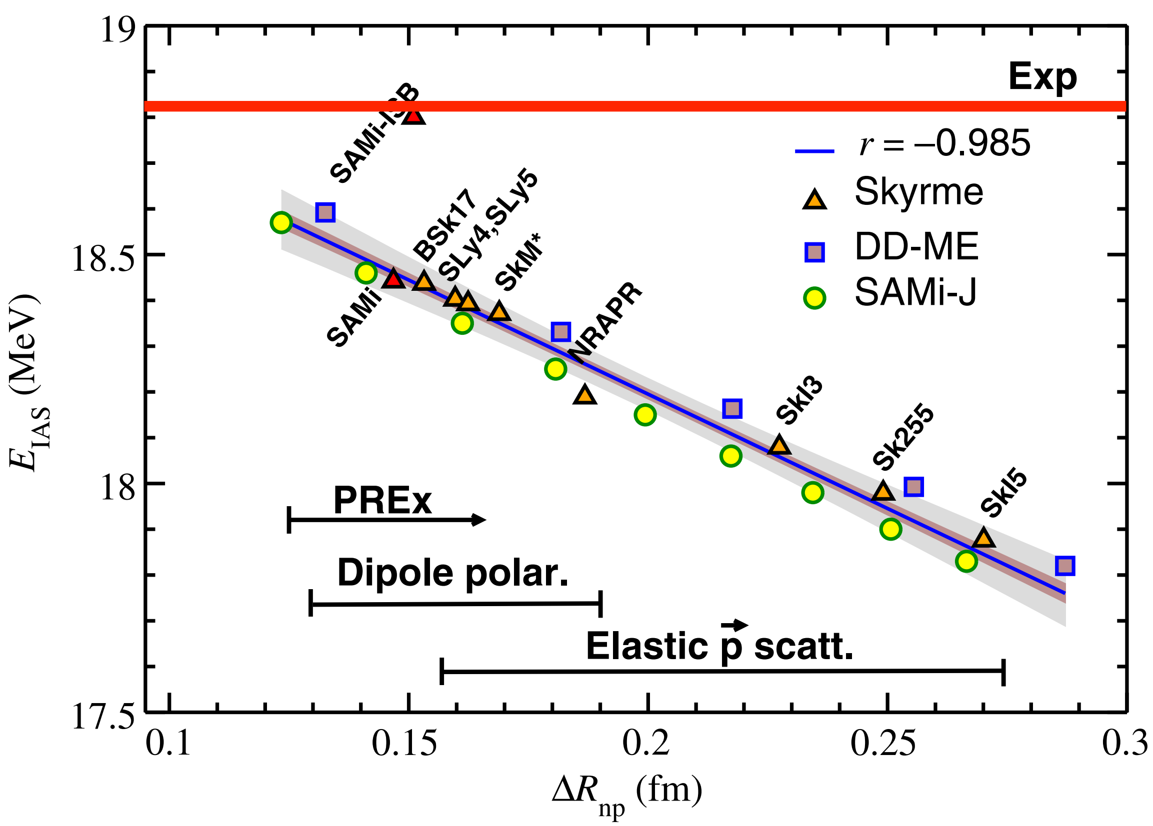


30 ≤ J ≤ 35 MeV
20 ≤ L ≤ 66 MeV

Nuclear Symmetry Energy and the Breaking of the Isospin Symmetry

PHYSICAL REVIEW LETTERS **120**, 202501 (2018)
X. Roca-Maza, G. Colò, and H. Sagawa

Charge-exchange RPA results for the IAS excitation energy in ^{208}Pb



	E_{IAS} (MeV)	Correction (keV)
No corrections	18.31	
Exact Coulomb exchange	18.41	+100
n/p mass difference	18.44	+30
Electromagnetic spin orbit	18.45	+10
Finite-size effects	18.40	−50
Vacuum polarization (V_{ch})	18.53	+130
Isospin symmetry breaking	18.80	+270

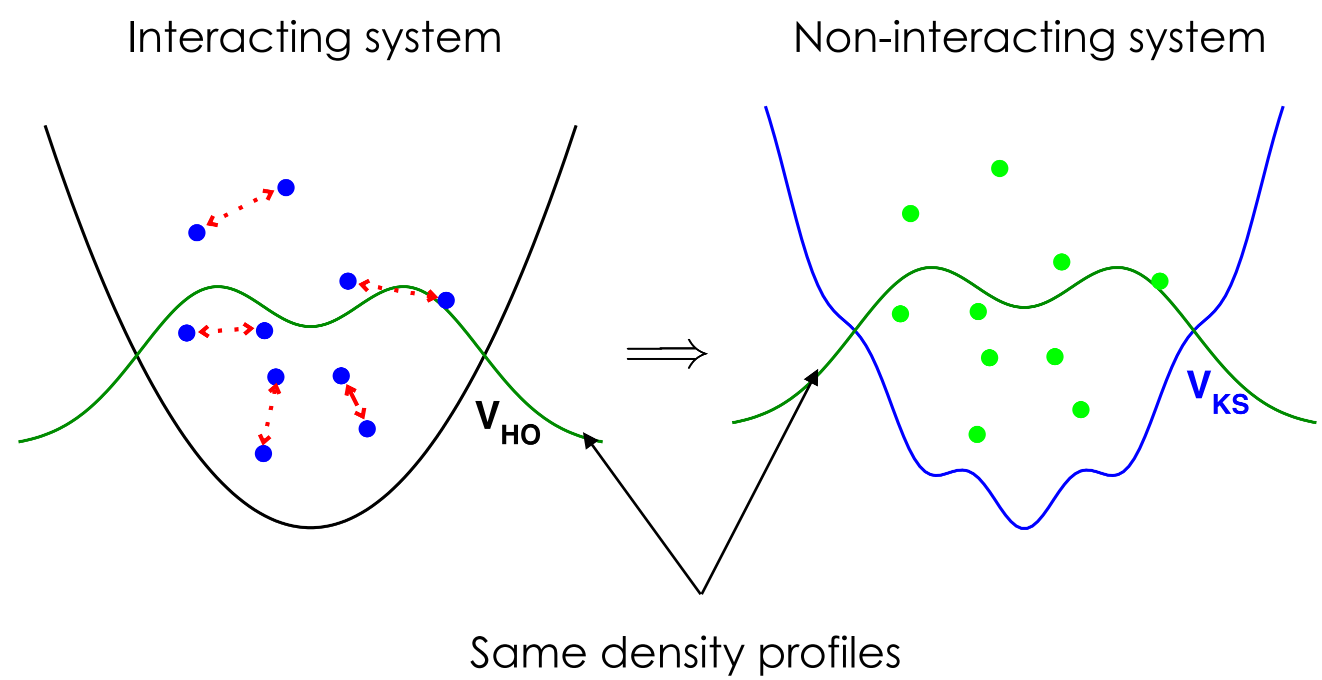
$$V_{\mathrm{CSB}}(\vec{r}_1,\vec{r}_2) \equiv \frac{1}{4}[\tau_z(1)+\tau_z(2)]s_0(1+y_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2),$$

$$V_{\mathrm{CIB}}(\vec{r}_1,\vec{r}_2) \equiv \frac{1}{2}\tau_z(1)\tau_z(2)u_0(1+z_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2).$$

New functional: SAMi-ISB

Nuclear Energy Density Functionals

Kohn-Sham DFT



For any interacting system, there exists a local single-particle (Kohn-Sham) potential $v_s(r)$, such that the exact ground-state density of the interacting system equals the ground-state density of the auxiliary problem:

$$n(\mathbf{r}) = n_s(\mathbf{r}) \equiv \sum_i^{occ} |\phi_i(\mathbf{r})|^2$$

The single-particle orbitals are solutions of the Kohn-Sham equations:

$$\left[-\nabla^2/2 + v_s(\mathbf{r})\right] \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

The Hohenberg-Kohn functional is partitioned:

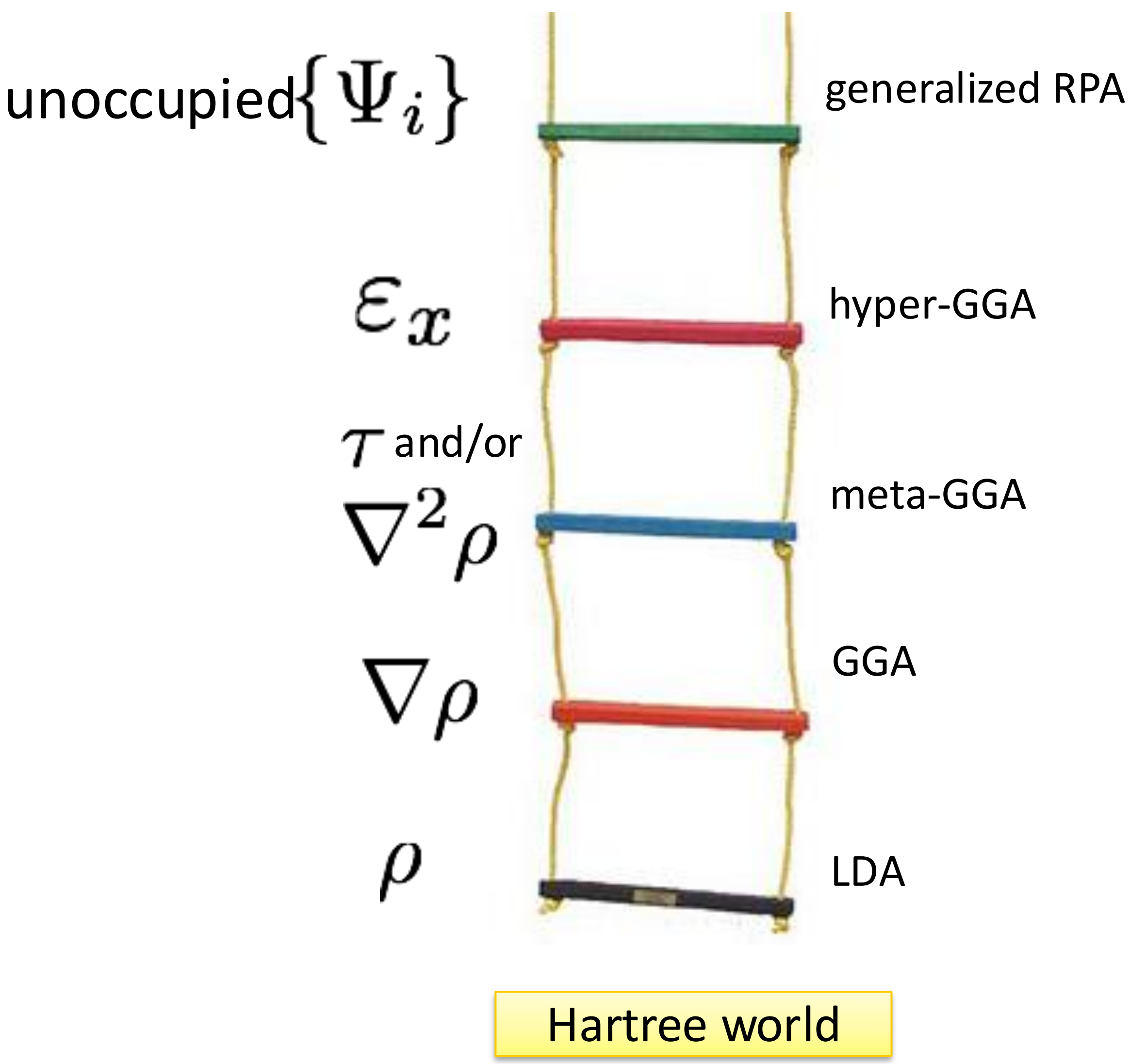
$$F[n] = T_s[n] + U[n] + E_{xc}[n]$$

Kinetic energy of the non-interacting system

Hartree term

Exchange-correlation energy which, by definition, includes everything else!

Ladder of DFT approximations for E_{xc}



ADVANCES IN PHYSICS: X
2020, VOL. 5, NO. 1, 1740061
https://doi.org/10.1080/23746149.2020.1740061

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Nuclear density functional theory

G. Colò [a,b]

Direct Kohn-Sham

$$E[\rho] = T + F + V_{\text{ext}}$$

Exact but unknown! Approximated by a functional of powers and gradients of ground-state nucleon densities and currents.

$$v[\rho] \equiv \frac{\delta F}{\delta \rho} \Rightarrow \text{KS equation} \Rightarrow \rho(\mathbf{r}) = \sum_\alpha \phi_\alpha^*(\mathbf{r})\phi_\alpha(\mathbf{r}).$$

$$E[\rho] \quad \rightarrow \quad v[\rho] \quad \rightarrow \quad \rho$$

Inverse Kohn-Sham

Starting from a given density (experimental), the effective potential and, eventually, energy density functional are deduced.

$$\rho \quad \rightarrow \quad v[\rho] \quad \rightarrow \quad E[\rho]$$

D2P P2E

Is the IKS problem well posed?

A problem is well-posed if a solution exists, is unique, and continuously changes with the input. If a problem is not well-posed, then it is ill-posed!

Nuclear Inverse Kohn-Sham

PHYSICAL REVIEW C **101**, 024315 (2020)

G. Accorto, P. Brandolini, F. Marino, A. Porro, A. Scalesi, G. Colò, X. Roca-Maza, and E. Vigezzi

First step in the nuclear inverse Kohn-Sham problem: From densities to potentials

PHYSICAL REVIEW C **103**, 044304 (2021)

Giacomo Accorto, Tomoya Naito (内藤智也), Haozhao Liang (梁豪兆), Tamara Nikšić, and Dario Vretenar

Nuclear energy density functionals from empirical ground-state densities

PHYSICAL REVIEW C **105**, 034309 (2022)

A. Liardi, F. Marino, G. Colò, X. Roca-Maza, and E. Vigezzi

Complete solution to the inverse Kohn-Sham problem: From the density to the energy

1. Density-to-potential

CONSTRAINED-VARIATIONAL METHOD

$$T[\{\phi_\alpha(\mathbf{r})\}] = -\frac{\hbar^2}{2m}\sum_{\alpha=1}^{N}\int d\mathbf{r}\; \phi^*_\alpha(\mathbf{r})\nabla^2\phi_\alpha(\mathbf{r}).$$

… minimize under the constraints: (i) orthonormality of s.p. orbitals,
(ii) the density of the system equals the target density

⇒ cost functional:

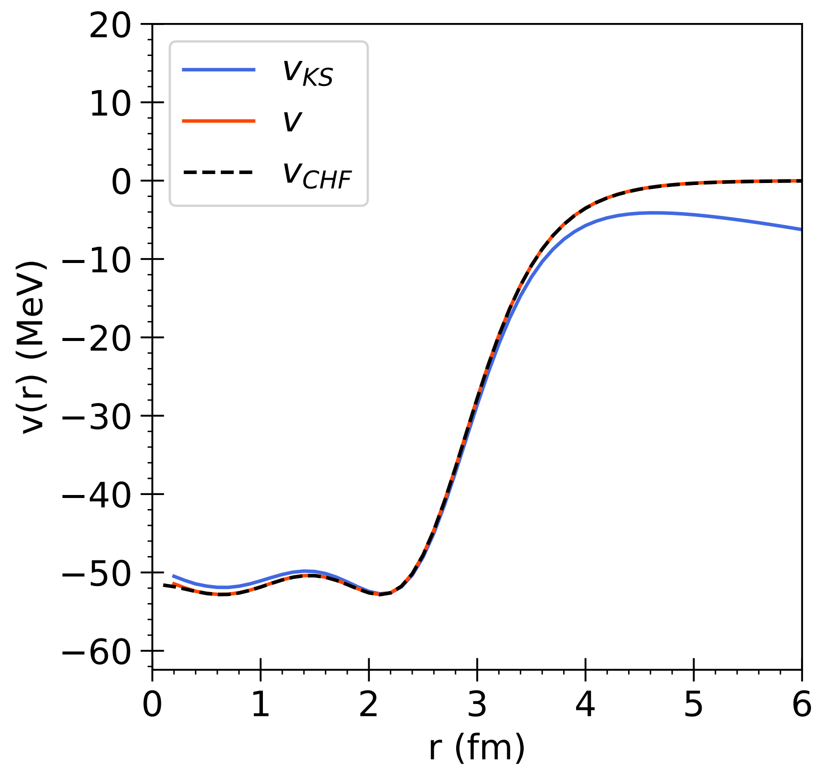
$$J[\{\phi_\alpha(\mathbf{r})\}; v_{\mathrm{KS}}(\mathbf{r}), \{\epsilon_{\alpha\beta}\}] = T[\{\phi_\alpha(\mathbf{r})\}] + \int d\mathbf{r}\; v_{\mathrm{KS}}(\mathbf{r})[\rho(\mathbf{r}) - \tilde{\rho}(\mathbf{r})] - \sum_{\alpha<\beta}\epsilon_{\alpha\beta}\left(\int d\mathbf{r}\; \phi^*_\alpha(\mathbf{r})\phi_\beta(\mathbf{r}) - \delta_{\alpha\beta}\right).$$

Kohn-Sham potential → Lagrange multiplier associated with the density constraint.

⇒ Euler-Lagrange equations for *J*:

$$-\frac{\hbar^2}{2m}\nabla^2\phi_\alpha(\mathbf{r}) + v_{\mathrm{KS}}(\mathbf{r})\phi_\alpha(\mathbf{r}) = \sum_{\beta}\epsilon_{\alpha\beta}\phi_\beta(\mathbf{r}).$$

16O → the potential derived from ρ_μ by the IKS method (v_{KS}), the CHF potential v_{CHF} and $v = v_{KS,\mu} - \mu r^2$ are compared for $\mu = -0.2$ MeV fm^{-2}.



2. Potential-to-energy functional

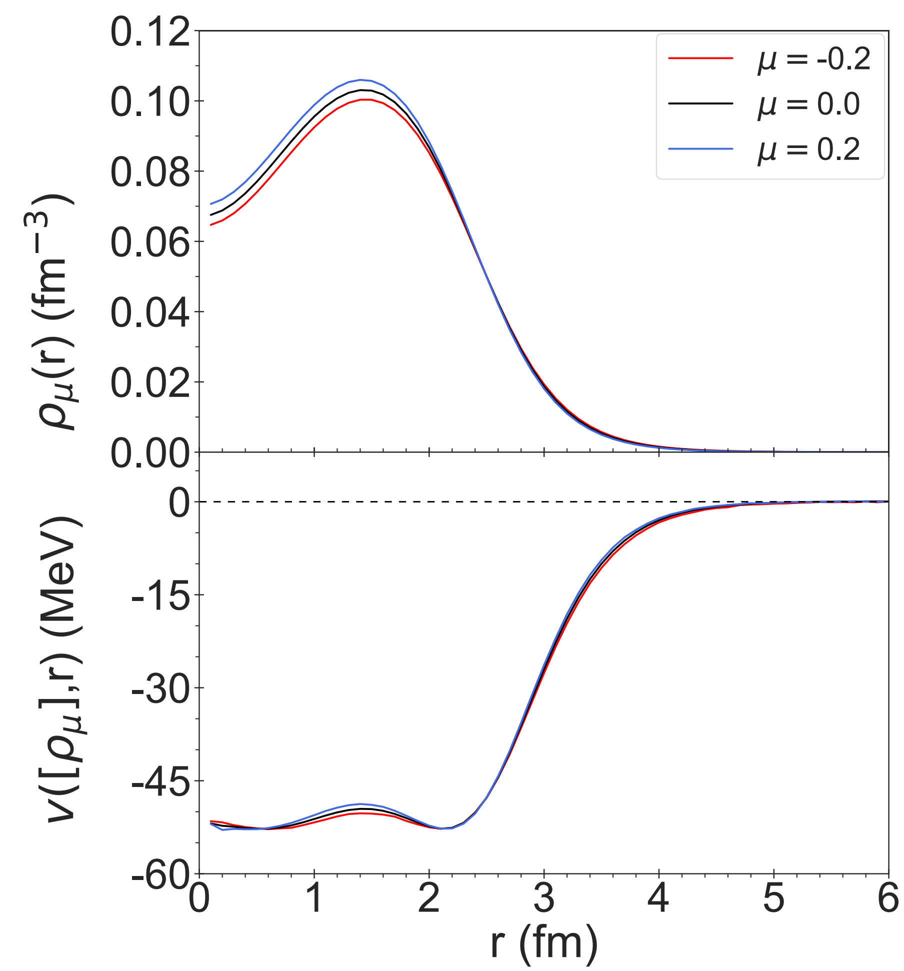
THE LINE INTEGRATION FORMULA

If one knows the effective potential v[ρ] along a path of densities, then the corresponding change in the energy functional can be reconstructed.

⇒ one-parameter family of densities: $\rho_t(\mathbf{r}) \qquad A \leqslant t \leqslant B.$

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

16O → monopole constrained densities ρ_μ and the corresponding potentials $v = v_{KS,\mu} - \mu r^2$, for $\mu = -0.2, 0, 0.2$ MeV fm^{-2}.



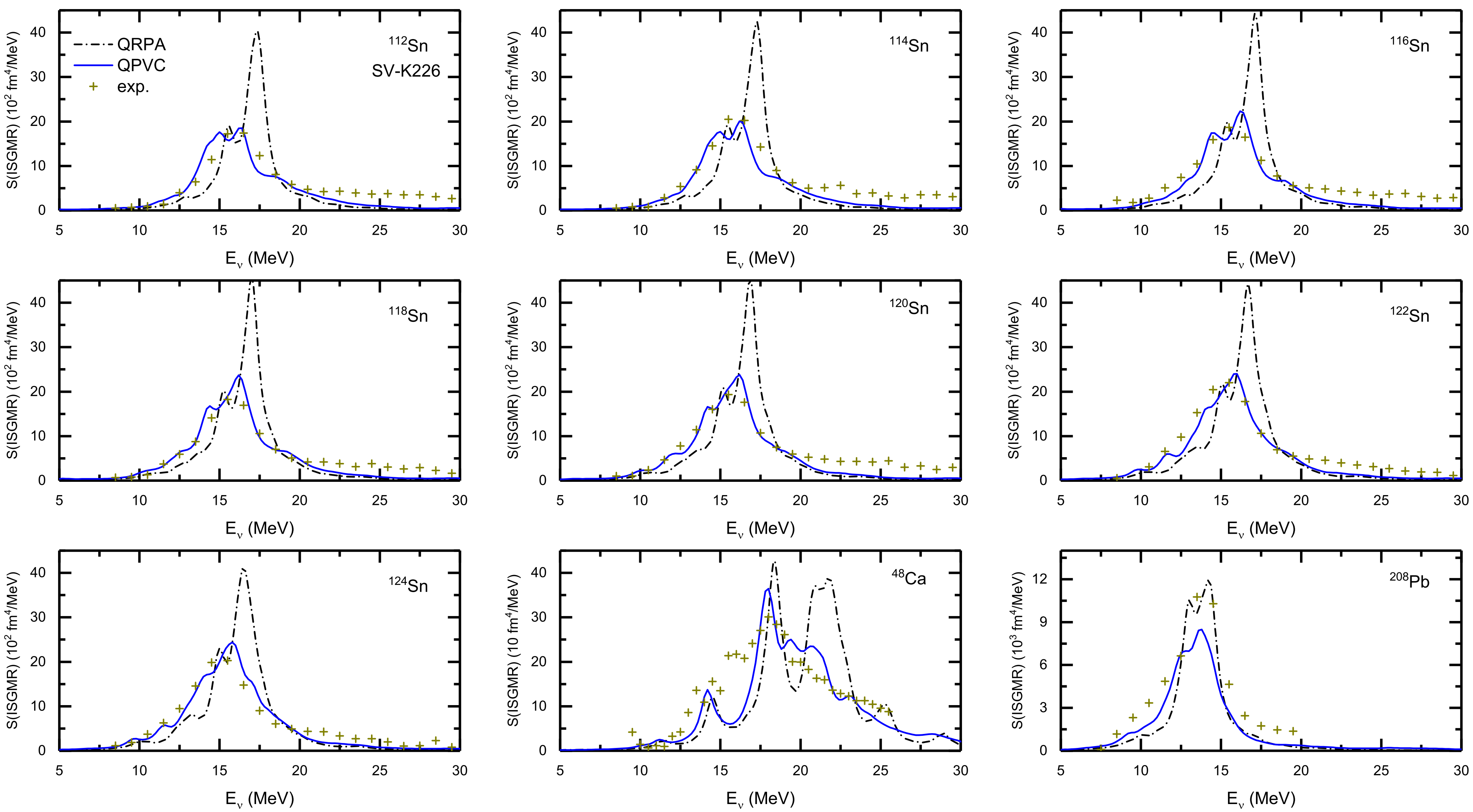
PHYSICAL REVIEW LETTERS

Toward a Unified Description of Isoscalar Giant Monopole Resonances in a Self-Consistent Quasiparticle-Vibration Coupling Approach

Z. Z. Li (李征征), Y. F. Niu (牛一斐), and G. Colò
Phys. Rev. Lett. **131**, 082501 – Published 23 August 2023

Why is tin so soft?

QRPA + QPVC calculation of ISGMR in Ca, Sn and Pb → coupling with phonons J^{π} = 0+, 1-, 2+, 3-, 4+, 5- (E < 30 MeV).



Simultaneous description of ISGMR in Ca, Sn and Pb ⇒ $K_\infty \approx 230$ MeV.

Generalized time-dependent generator coordinate method

Li, Vretenar, Nikšić, Zhao, Meng, Phys. Rev. C **108**, 014321 (2023).

The nuclear wave function: $|\Psi(t)\rangle = \sum_{\boldsymbol{q}} f_{\boldsymbol{q}}(t)|\Phi_{\boldsymbol{q}}(t)\rangle \quad \Longrightarrow \quad i\hbar\partial_t|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$

collective coordinate

$\Longrightarrow$ equation of motion for the weight functions: $\sum_{\boldsymbol{q}} i\hbar\mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t)\partial_t f_{\boldsymbol{q}}(t) + \sum_{q} \mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t) = \sum_{q} \mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) f_{\boldsymbol{q}}(t)$

...time-dependent kernels:

$$\begin{cases} \mathcal{N}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\Phi_{\boldsymbol{q}}(t)\rangle, \\ \mathcal{H}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|\hat{H}|\Phi_{\boldsymbol{q}}(t)\rangle, \\ \mathcal{H}^{MF}_{\boldsymbol{q}'\boldsymbol{q}}(t) = \langle\Phi_{\boldsymbol{q}'}(t)|i\hbar\partial_t|\Phi_{\boldsymbol{q}}(t)\rangle, \end{cases}$$

The time-dependent generator states are independent TDDFT trajectories in the space of collective coordinates.

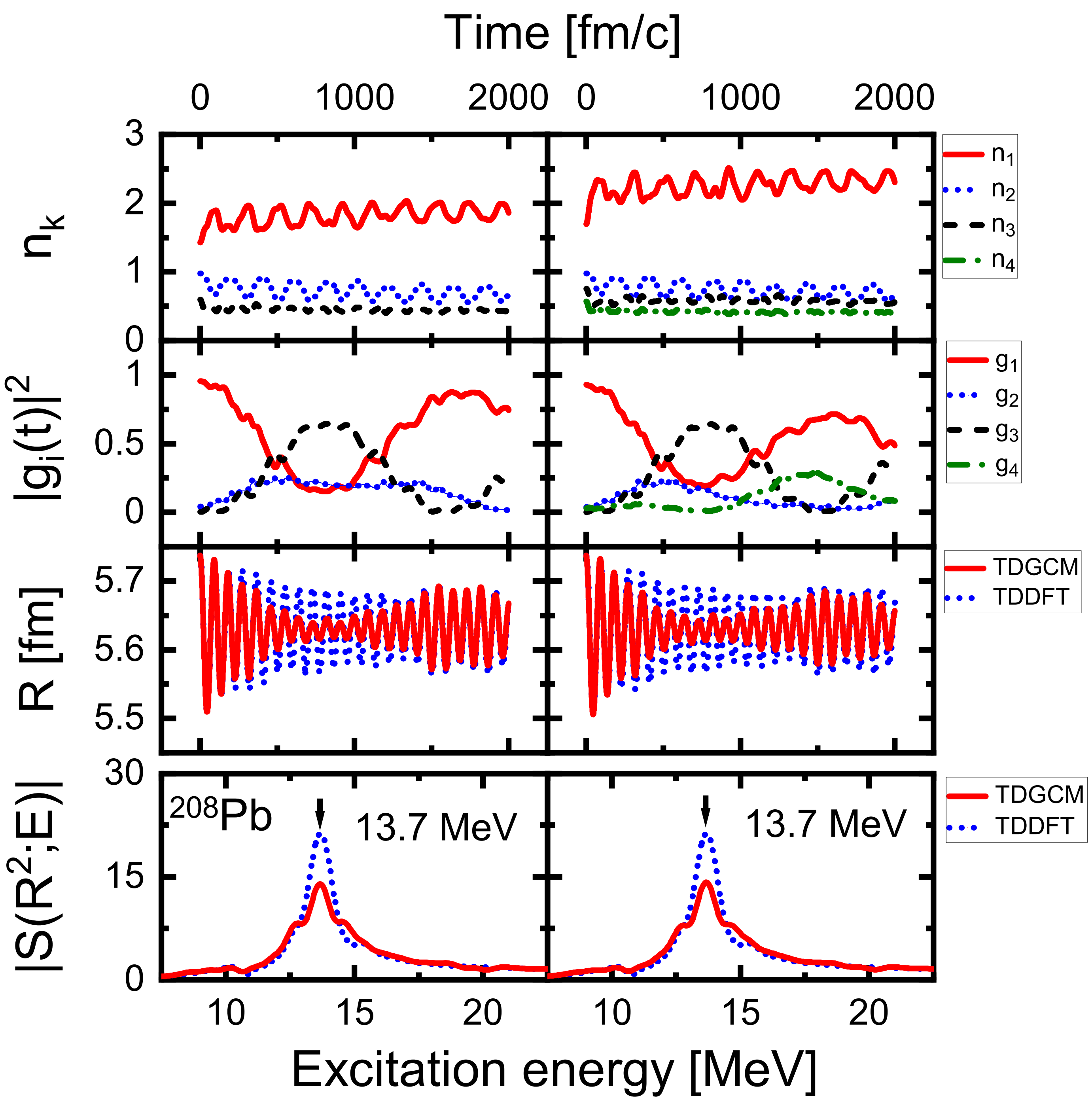
...collective wave function: $g = \mathcal{N}^{1/2} f$

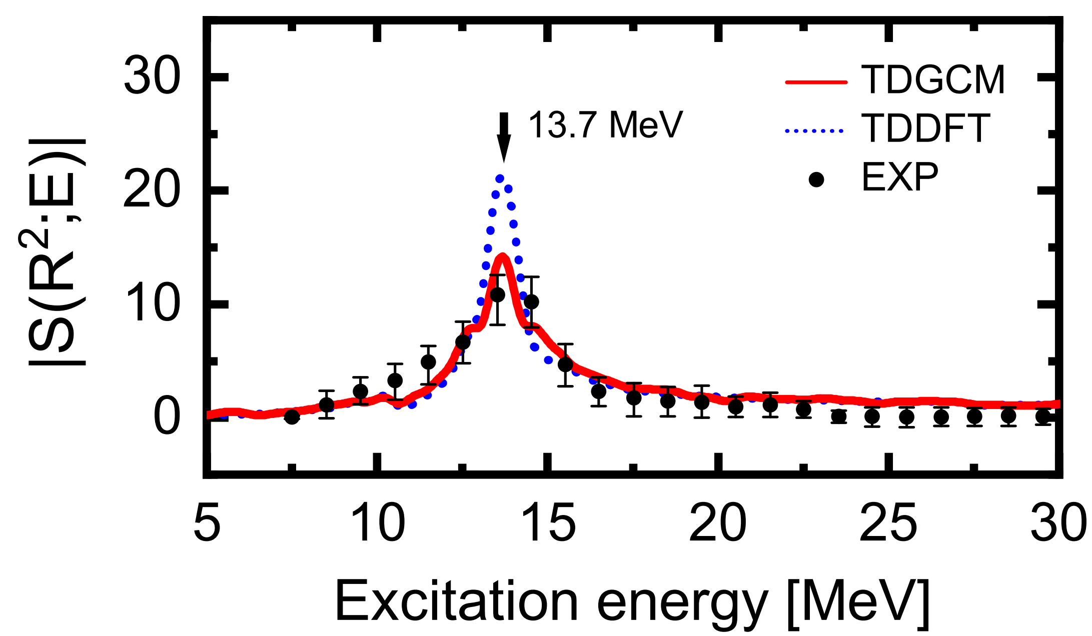
$$\boxed{i\hbar\dot{g} = \mathcal{N}^{-1/2}(H - H^{MF})\mathcal{N}^{-1/2} g + i\hbar\dot{\mathcal{N}}^{1/2}\mathcal{N}^{-1/2} g.}$$

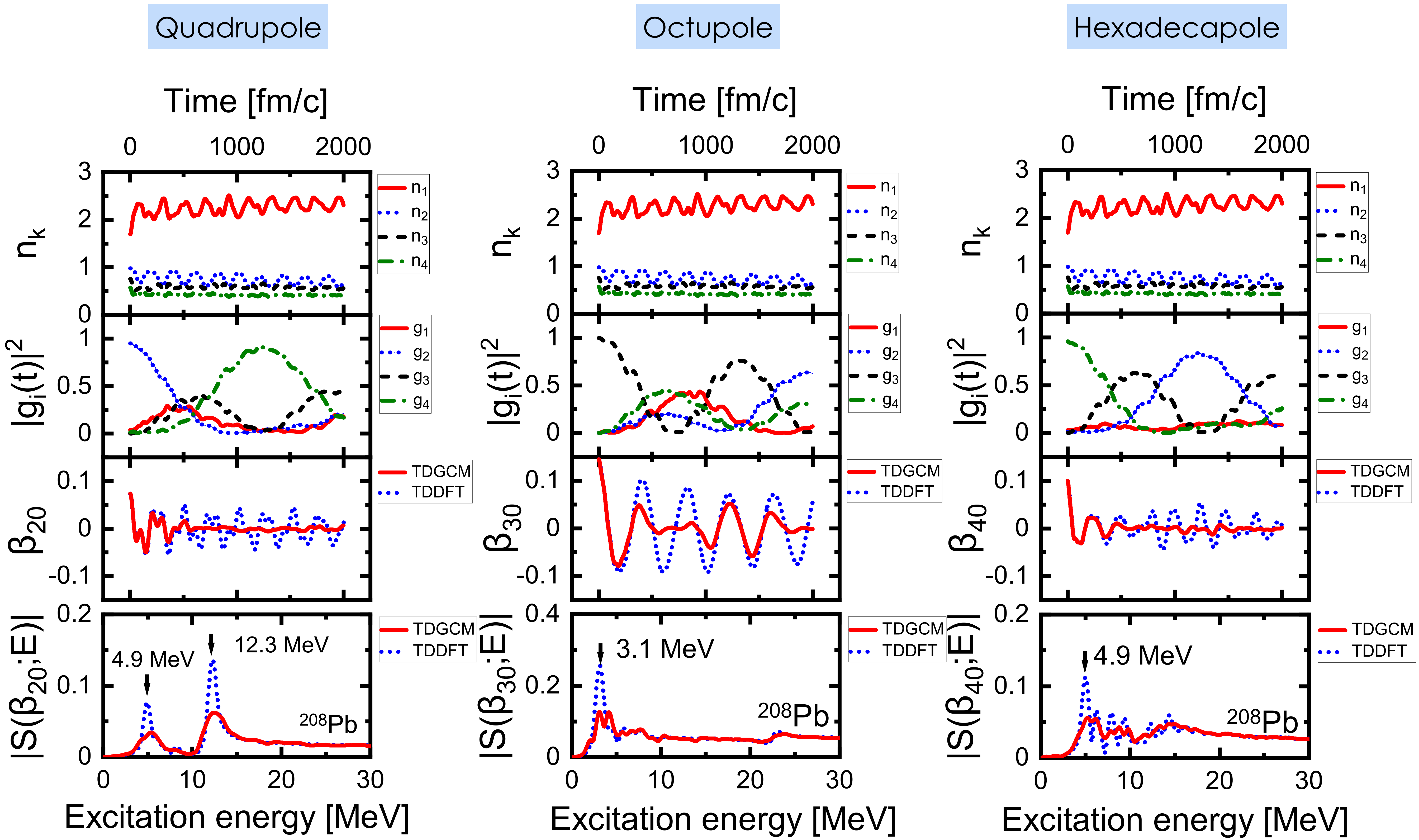
Collective Vibrations of ^{208}Pb: mode coupling

R_{init} = 5.737 fm, $\beta_{20,init}$ = 0.074, and $\beta_{30,init}$ = 0.145.

R_{init} = 5.737 fm, $\beta_{20,init}$ = 0.074, $\beta_{30,init}$ = 0.145 and $\beta_{40,init}$ = 0.1.







R_{init} = 5.737 fm, $\beta_{20,\mathrm{init}}$ = 0.074, $\beta_{30,\mathrm{init}}$ = 0.145 and $\beta_{40,\mathrm{init}}$ = 0.1.