Giant resonances in the Skyrme-Hartree-Fock theory

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COMEX05, Krakow 2015

Acknowledgements

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Support: BMBF contract 05P12RFFTG, DFG Re-322/12-1

Outline

1. Formal framework
   - The Skyrme energy-density functional
   - Observables
   - Optimization of model parameters by least-squares fits

2. Results
   - RPA: convergence and 2ph effects
   - Giant resonances and nuclear matter parameters (NMP)
   - GDR – trends with mass number
   - Isovector dipole strength at low *E*

3. Conclusions

Formal framework

The Skyrme energy-density functional (here only time even densities)

$$E_{\text{tot}} = \int d^3r\, \mathcal{E}_{\text{Skyrme}}(\rho, \tau, \mathbf{J})$$

$$\begin{aligned}
& \tfrac{1}{2}B_0 \quad \rho^2 && + \tfrac{1}{2}B_0' \quad \tilde{\rho}^2 \\
+ & \tfrac{1}{2}B_3 \quad \rho^{2+\alpha} && + \tfrac{1}{2}B_3' \quad \tilde{\rho}^2\rho^\alpha \\
+ & B_1 \quad \rho\tau && + B_1' \quad \tilde{\rho}\tilde{\tau} \\
+ & \tfrac{1}{2}B_2 \quad (\nabla\rho)^2 && + \tfrac{1}{2}B_2' \quad (\nabla\tilde{\rho})^2 \\
+ & \tfrac{1}{2}B_4 \quad \rho\nabla\mathbf{J} && + \tfrac{1}{2}B_4' \quad \tilde{\rho}\nabla\tilde{\mathbf{J}}
\end{aligned}$$

isoscalar *isovector*

density $\rho(r) = \sum_\alpha v_\alpha^2 |\varphi_\alpha|^2$

kinetic density $\tau(r) = \sum_\alpha v_\alpha^2 |\nabla\varphi_\alpha|^2$

spin-orbit dens. $\mathbf{J}(r) = -\mathrm{i}\sum_\alpha v_\alpha^2 \varphi_\alpha^\dagger \nabla\times\sigma\varphi_\alpha$

total & difference $\underbrace{\rho = \rho_n + \rho_p}_{\text{isoscalar}},\ \underbrace{\tilde{\rho} = \rho_n - \rho_p}_{\text{isovector}}$

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$$E_{\rm tot} = E_{\rm kin} + \int d^3r\,\mathcal{E}_{\rm Skyrme}(\rho,\tau,\mathbf{J}) + \int d^3r\,\mathcal{E}_{\rm pair}(\chi,\rho) + E_{\rm Coul} - E_{\rm corr}$$

$$\sum_\alpha \frac{(\varphi_\alpha|\hat{\mathbf{p}}^2|\varphi_\alpha)}{2m_N}$$

kinetic energy

correlations from low energy modes: c.m., rotation, vibrat.

Coulomb en. (exchange = Slater appr.)

$$\left(V_{\rm p}^{\rm pair}\chi_{\rm p}^2 + V_{\rm n}^{\rm pair}\chi_{\rm n}^2\right)\left(1 - \frac{\rho}{\rho_{\rm pair}}\right)$$

pairing functional

only surface effects

to define open shell nuclei

$$\begin{aligned}
& \tfrac{1}{2}B_0\,\rho^2 && + \tfrac{1}{2}B_0'\,\tilde{\rho}^2 \\
+ & \tfrac{1}{2}B_3\,\rho^{2+\alpha} && + \tfrac{1}{2}B_3'\,\tilde{\rho}^2\rho^\alpha \\
+ & B_1\,\rho\tau && + B_1'\,\tilde{\rho}\tilde{\tau} \\
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pair density $\chi(r) = \sum_\alpha u_\alpha v_\alpha|\varphi_\alpha|^2$

pairing amplit. u_α, v_α

total & difference $\underbrace{\rho = \rho_n + \rho_p}_{\text{isoscalar}},\ \underbrace{\tilde\rho = \rho_n - \rho_p}_{\text{isovector}}$

free parameters: $\underbrace{B_0, B'_0, B_1, B'_1, B_2, B'_2, B_3, B'_3, \alpha,}$ $B_4, B'_4, V_{\rm p}^{\rm pair}, V_{\rm n}^{\rm pair}, \rho_{\rm pair}$

$\leftrightarrow$ nuclear matter parameters (NMP)

Observables

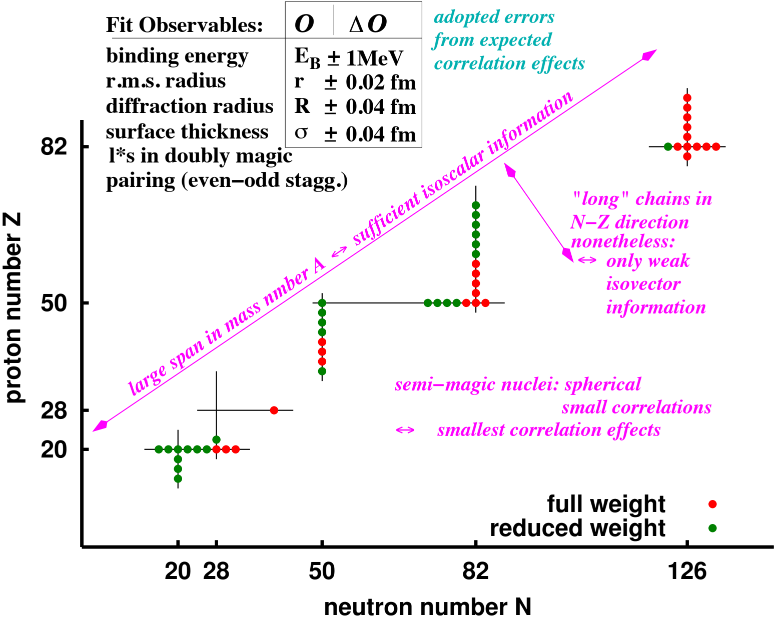
The nuclear matter parameters (NMP)

given $E/A(\rho) =$ energy per particle in symmetric nuclear matter (ρ = total density)
this allows to define basic properties at equilibrium:

$E/A_{\rm eq}$	binding energy per particle at equilibrium point
$\rho_{\rm eq}$	equilibrium density
$K = 9\rho_0^2\partial_\rho^2\frac{E}{A}$	incompressibility (isoscalar static response)
$\frac{m^*}{m}$	effective mass (isoscalar dynamic response)
J	symmetry energy (isovector static response)
$L = 3\rho_0\partial_\rho a_{\rm sym}$	slope of symmetry energy
$\kappa_{\rm TRK}$	TRK sum rule enhancement $\leftrightarrow$ isovector $\frac{m_1^*}{m}$ (dynamic response)
$a_{\rm surf}$	surface energy
$a_{\rm surf,sym}$	surface symmetry energy

these 9 NMP are equivalent to parameters of SHF functional (except l*s & pairing)

Ground state properties in the pool of fit data



Further observables

Response properties in ^{208}Pb

- giant resonances: monopole (GMR), quadrupole (GQR), dipole (GDR)
- dipole polarizability $\alpha_D = \int_0^\infty \mathrm{d}\omega\, S_D(\omega)\, \omega^{-1}$ in ^{208}Pb

Other:

- neutron skin $r_n - r_p$ in ^{208}Pb
- neutron "equation of state" (EoS) $E/N_{\mathrm{neut}}(\rho)$
- binding energy E_B for exotic nuclei (super-heavy 120/182; neutron rich ^{148}Sn)

Description of excitation spectra $\leftrightarrow$ RPA and beyond

RPA: small amplitude limit of time-dependent Hartree-Fock

eigenmodes = optimized 1*ph* excitation operators $\hat{C}_N^\dagger = \sum_\nu b_\nu \hat{A}_\nu$

$$\hat{A}_\nu \in \{ \underbrace{\hat{a}^\dagger \hat{a}, \hat{a}\hat{a}^\dagger}_{E<30\ \mathrm{MeV}}, \underbrace{r^{L+n} Y_{LM}, j_L(qr) Y_{LM}, [\hat{H}, r^{L+n} Y_{LM}], [\hat{H}, j_L(qr) Y_{LM}]}_{\text{global couplings, high } E} \}$$

RPA equations from variational formulation: $\delta_{b_\nu^*} \dfrac{\langle [\hat{C}_N, [\hat{H}, \hat{C}_N^\dagger]] \rangle}{\langle [\hat{C}_N, \hat{C}_N^\dagger] \rangle} = 0$

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numerically handled by commutator algebra on the grid

+phonons: couple basis states $\hat{A}_\nu$ to few low-lying & strong $\hat{C}^\dagger_S$

basis of 1*ph* & 2*ph* operators: $\tilde{C}^\dagger_{\tilde{N}} = \sum_\nu b_\nu \hat{A}_\nu + \sum_{\nu,S} b_{\nu,S} \hat{A}_\nu \hat{C}^\dagger_S$

approximations: residual interaction $\hat{V}_{\rm res}$ from RPA (?: 1*ph*-1*ph* used for 1*p*1*p*-1*ph*)
exchange terms in $\hat{V}_{\rm res}$ neglected (?: Pauli principle)

Optimization of model parameters

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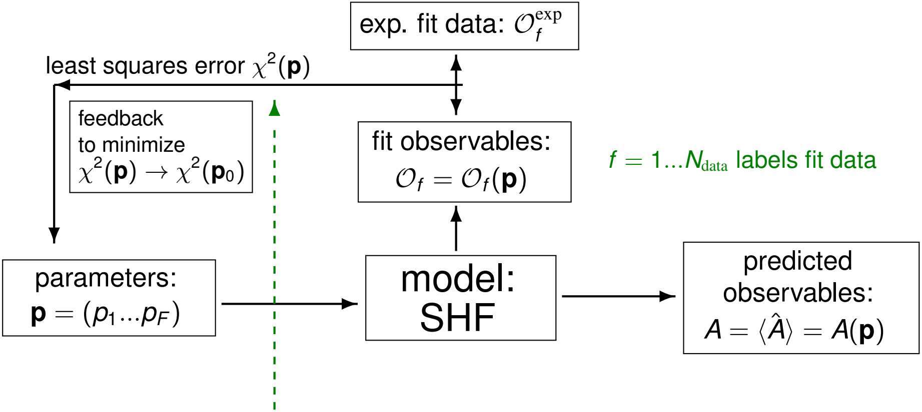
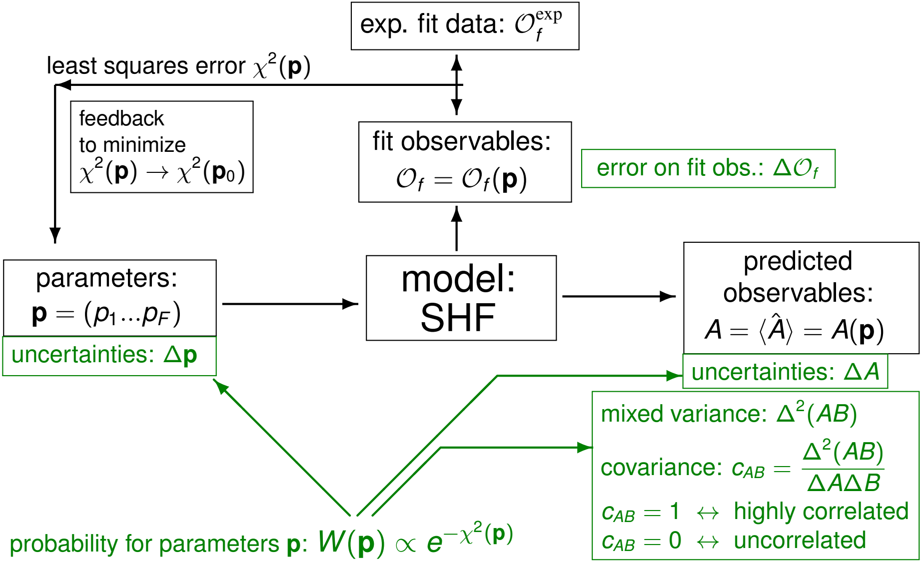


$$\chi^2(\mathbf{p}) = \sum_{f=1}^{N_{\rm data}} \frac{\left(\mathcal{O}_f(\mathbf{p}) - \mathcal{O}_f^{\rm exp}\right)^2}{\Delta \mathcal{O}_f^2}$$

adopted error $\Delta\mathcal{O}_f$: $\chi^2(\mathbf{p}_0) = N_{\rm data} - N_{\rm params}$

Optimization of model parameters



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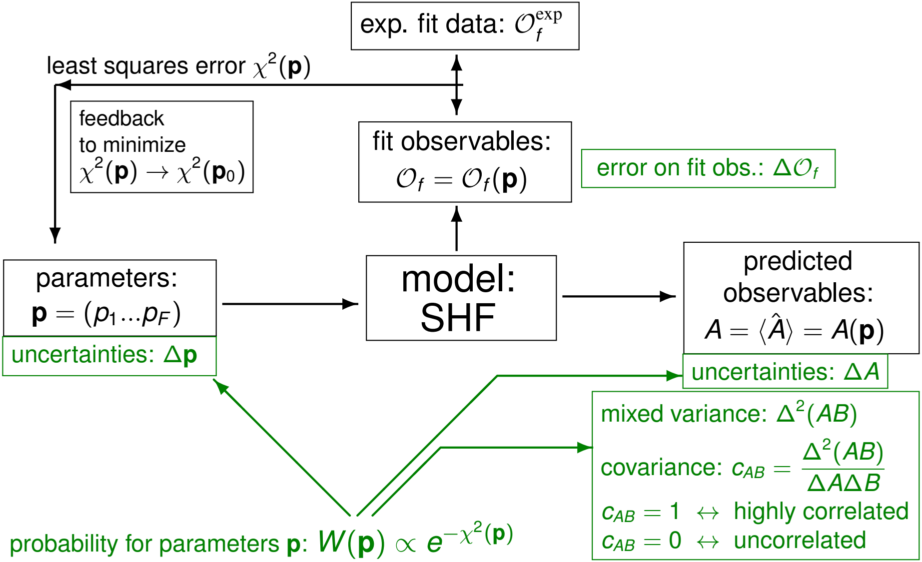
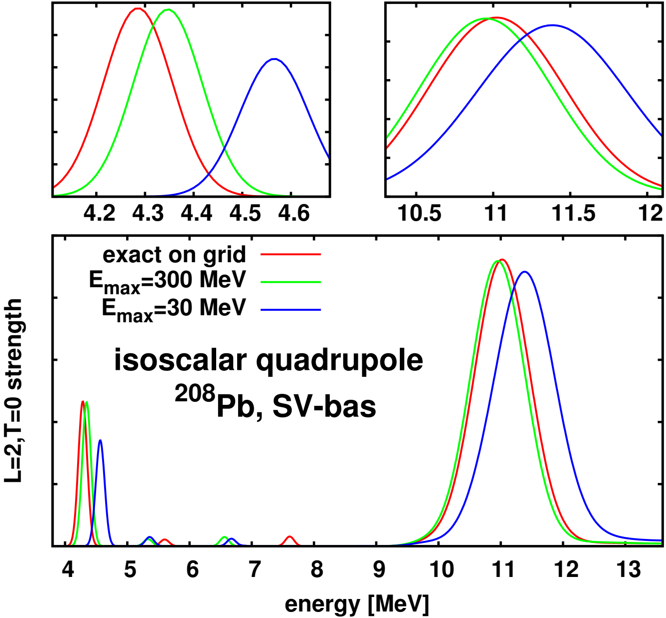


fit to g.s. data only = SV-min , fit to g.s. data + NMP = SV-bas

Results

RPA: convergence and 2ph effects

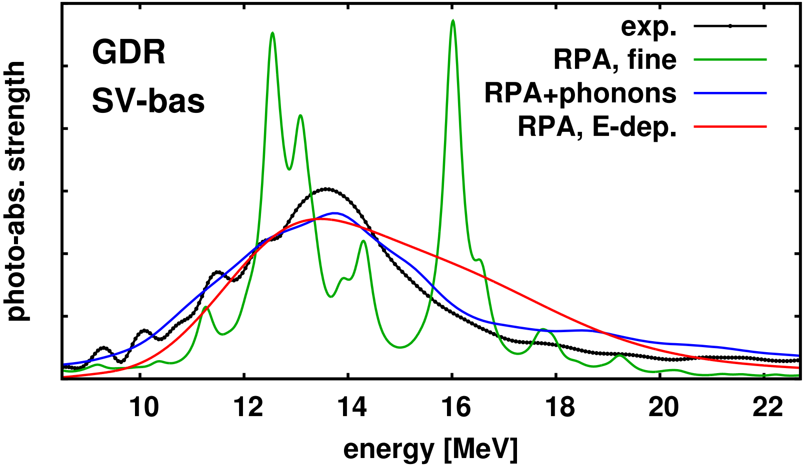
RPA phase space – example isoscalar quadrupole (L=2,T=0)



basis up to
$E_{\rm max} \approx 100$ MeV
suffices
for giant resonances

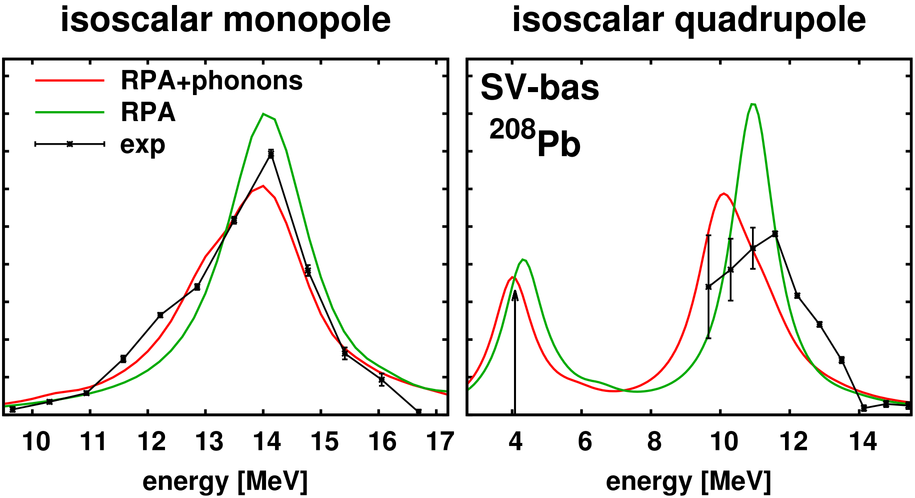
low-lying 2^+ states
more demanding

Giant dipole resonance (GDR) – collisional width



RPA, fine:	folding 0.2 MeV + escape width ⇒ proper region, unrealistic profile
RPA+phonons:	perfect peak position, perfect profile ↔ proper smoothing
RPA, E-dep.:	E-dependend folding width ⇒ acceptable model for collisional width

Isoscalar giant resonances (GMR & GQR) – phonon coupling

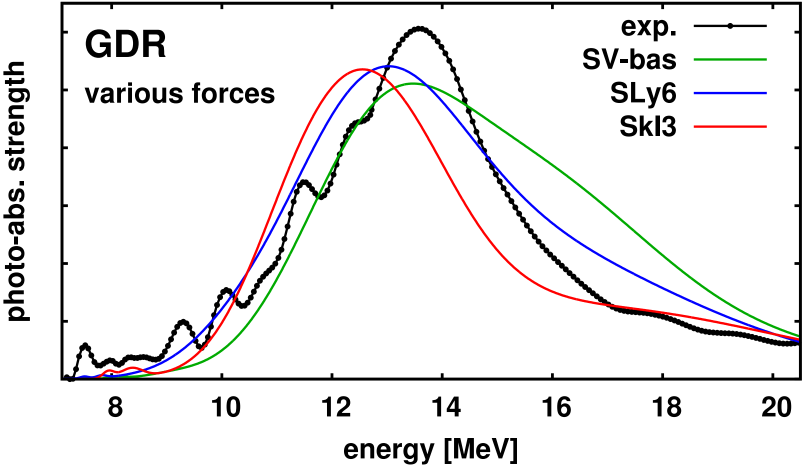


width again well reproduced by *E*-dependent folding
phonon coupling ⇒ some downshift of centroid: L=0&2 ↔ $\approx -0.5 MeV$

⟹ point not yet settled, remains open (uncertainty $0.5 MeV$) ⟶ continue with RPA

Giant resonances and nuclear matter parameters (NMP)

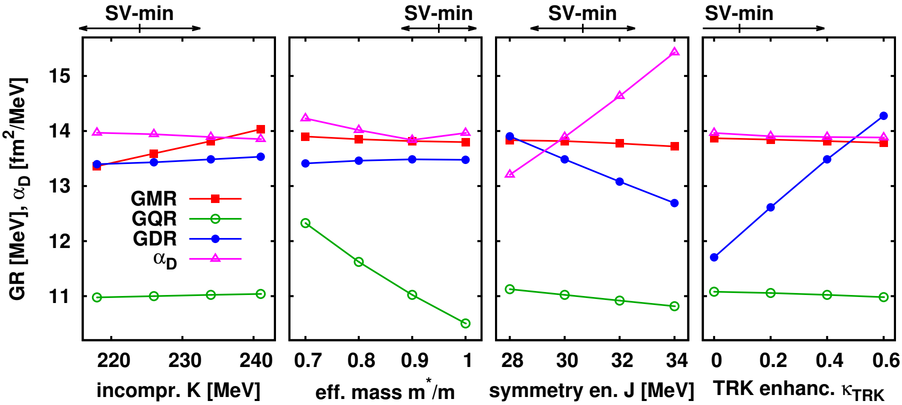
GDR – predictions from Skymre forces



take Skyrme forces with about the same quality for ground states
$\Longrightarrow$ very different predictions for giant resonances, particularly for GDR

$\longleftrightarrow$ dynamic response not well determined by ground state data
$\Longrightarrow$ use response properties to tune loosely fixed aspects of the SHF functional

Giant resonances and NMP – trend analysis



horizontal error bars ↔ uncertainties on NMP from fit to g.s. data only (SV-min)

each NMP is particularly sensitive to one response property (in ^{208}Pb):

$K \leftrightarrow$ GMR – $m^*/m \leftrightarrow$ GQR – $\kappa_{\mathrm{TRK}} \leftrightarrow$ GDR – $J \leftrightarrow \alpha_D$

$\Longrightarrow$ tune NMP to basic response properties (GMR, GQR, GDR, α_D)

$\Longrightarrow$ fit to g.s. data & with 4 fixed response properties (SV-bas)

$\Longrightarrow$ SV-bas accomodates more properties without sacrifices in quality on g.s. data

Giant resonances and NMP – covariance analysis

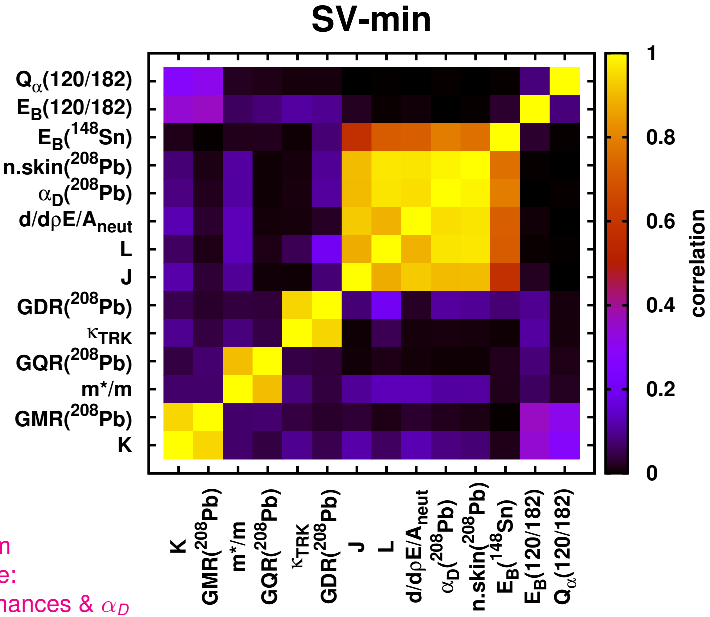
exotic nuclei

static isovector

dynamic isovector

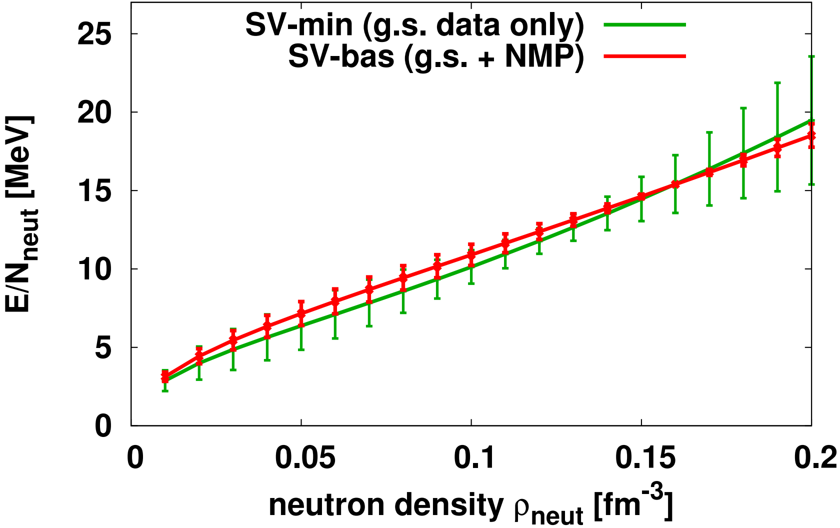
dynamic isoscalar

static isoscalar



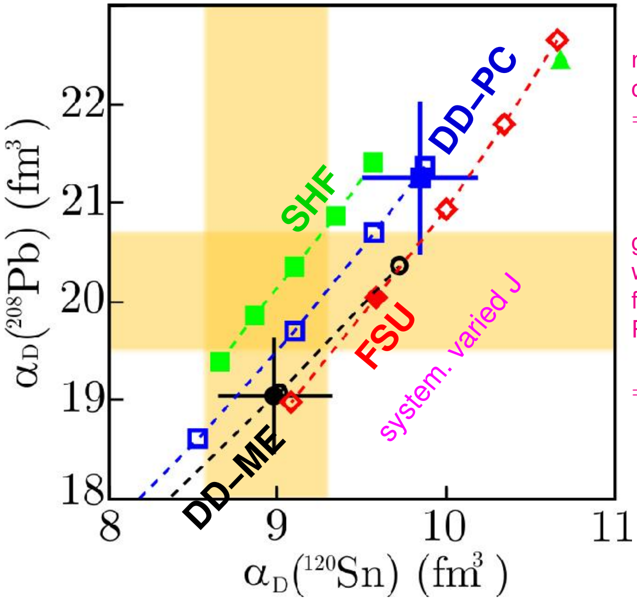
$\Longrightarrow$
covariances confirm
1:1 correspondence:
NMP $\leftrightarrow$ giant resonances & α_D

Consequences for extrapolation to neutron matter



information on response properties reduces uncertainty in extrapolations
for neutron equation-of-state particularly important: symmetry energy *J*

Dipole polarizability α_D as criterion



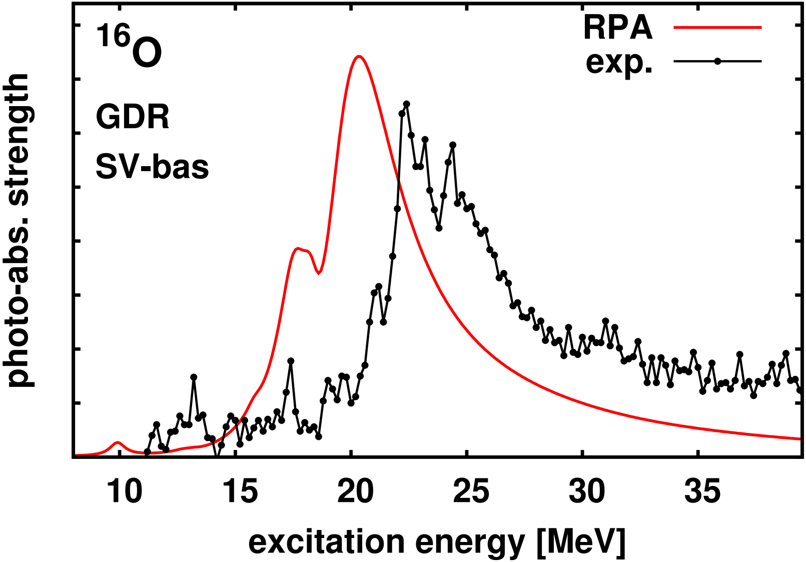
new high quality data for α_D:
comparison ^{208}Pb $\leftrightarrow$ ^{120}Sn
$\Rightarrow$ probe A-dependence of static isovector response

generate sets of forces with varied J for SHF and RMF (DD-PC, DD-ME, FSU)

$\Rightarrow$ SHF: fits "allowed" box
FSU: excluded by data
DD-ME: excluded by data
DD-PC: at the edge

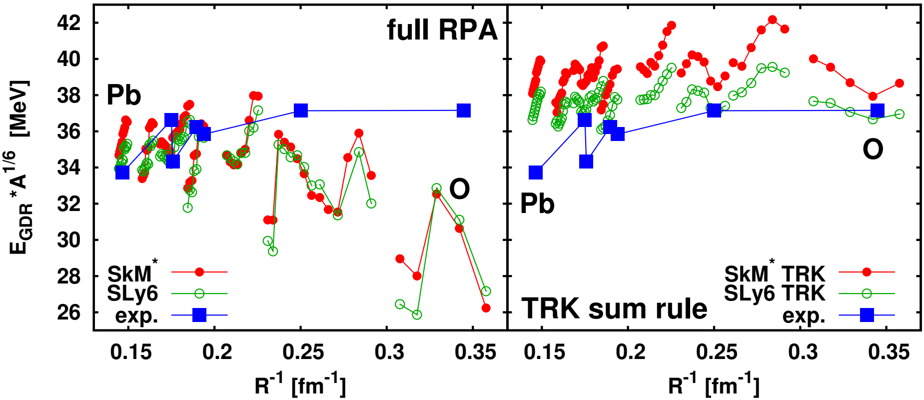
GDR – problem with light nuclei

GDR in ^{16}O



RPA from SHF yields too low GDR energy ↔ general problem for all SHF forces

GDR – trends with mass number

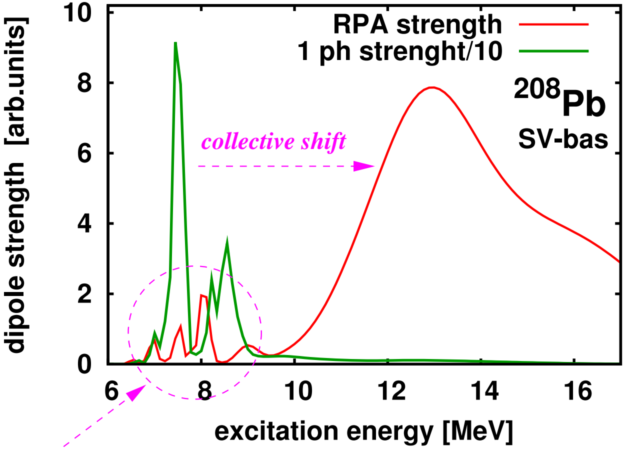


exp. = trend of GDR peaks $\propto A^{-1/6}$ $\overset{\lightning}{\longleftrightarrow}$ RPA = trend $\propto A^{-1/3}$ for all forces
$\Longrightarrow$ principle problem with density dep. of symmetry energy $J(\rho)$ or with $\kappa_{\mathrm{TRK}}(\rho)$
$\longleftrightarrow$ more flexible density dependence in SHF functional ? ($\leftrightarrow$ calibrate to $\alpha_D(A)$?)

noteworthy: TRK sum-rule has trend $\propto A^{-1/6}$ like experiment $\leftrightarrow$ meaning ?

Isovector dipole strength at low E

Dipole strength distribution in ^{208}Pb



1ph dipole strength gathers in narrow energy band

looks "resonance like" but is composed of several different 1ph states

RPA dipole strength collected in resonance peak (and somewhat fragmented to 1ph ...)

pygmy strength = "debris" from RPA recoupling reflects to a large extend the original 1ph structure

Detailed information $\longleftrightarrow$ transition formfactor

transition density: $\rho_{0\to N}(\mathbf{r}) = \langle\Phi_N|\hat{\rho}(\mathbf{r})|\Phi_0\rangle$ $\longleftrightarrow$ shows where transition is located

transition formfactor: $F_{0\to N}(\mathbf{q}) = \int d^3r\, e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}\, \rho_{0\to N}(\mathbf{r})$

$\longleftrightarrow$ shows preferred momentum transfer

in spherical nuclei sorting with respect to angular momentum L, M:

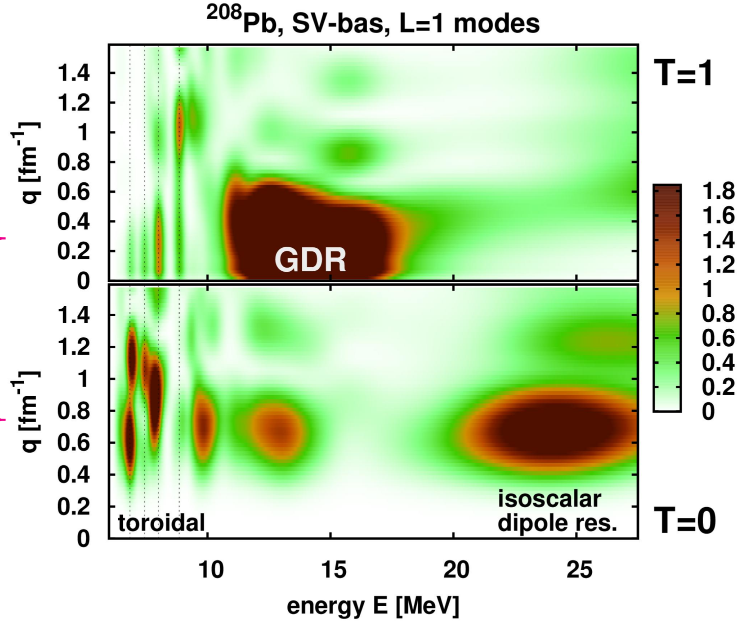
$$F^{(LM)}_{0\to N}(q) = \int d^3r\, j_L(qr)\, Y_{LM}(\Omega_{\mathbf{r}})\, \rho_{0\to N}(\mathbf{r}) = \langle\Phi_N|j_L(qr)\, Y_{LM}(\Omega_{\mathbf{r}})|\Phi_0\rangle$$

dipole momentum recovered in the limit $q \to 0$: $D^{(M)}_{0\to N} \propto \lim_{q\to 0} F^{(1M)}_{0\to N}(q)$

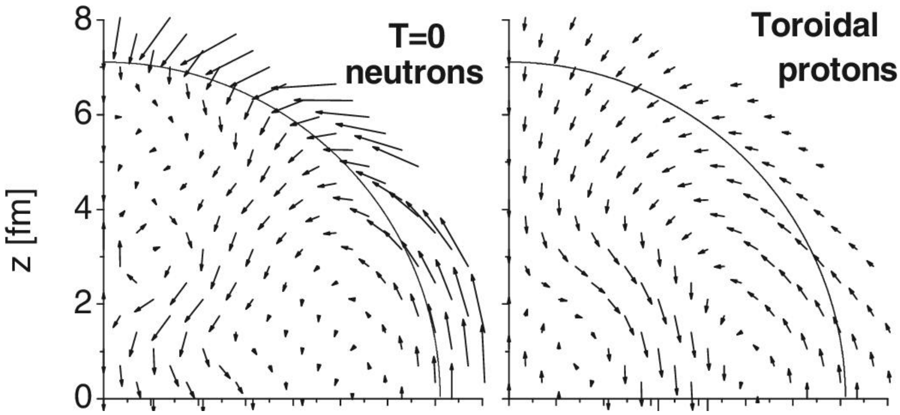
Transition formfactor for isoscalar & isovector dipole modes

low-lying isovector dipoles

driven by low-lying isoscalar modes (toroidal, compressional dipole)



Velocity map of isoscalar toroidal mode at 8.7 MeV



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Description of excitations (giant resonances etc):

RPA: commutator algebra, flexible basis expansion (1*ph* & local operators)
basis up to $E_{\mathrm{max}} \approx 100$ MeV for GR, more for low 2^+

+phonons: "phonons" = few low-lying RPA states with large strength
collisional broadening $\leftrightarrow$ can be simulated by *E*-dep. folding
slight down-shift of GMR&GQR $\leftrightarrow$ yet open details

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Giant resonances $\leftrightarrow$ nuclear matter parameters (NMP):

trends with NMP & covariances $\Longrightarrow$ nearly 1:1 correlation:

$$K \leftrightarrow \text{GMR} \ - \ m^*/m \leftrightarrow \text{GQR} \ - \ \kappa_{\rm TRK} \leftrightarrow \text{GDR} \ - \ J \leftrightarrow \alpha_D$$

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fits leave also leeway $\Rightarrow$ response properties can be accomodated

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GDR in light nuclei – problematic trend with mass number *A*:

$E_{\mathrm{GDR}}(^{16}\mathrm{O})$ too low for all resonable Skyrme forces
exp. trend $E_{\mathrm{GDR}} \propto A^{-1/6} \quad \longleftrightarrow \quad$ RPA trend $E_{\mathrm{GDR}} \propto A^{-1/3} \quad \lightning$
more (isovector) density dependence? – complex configurations (phonons)?

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Low-lying isovector dipole modes ("pygmy", range 7 MeV $< E <$ 10 MeV):

energy region where pure 1*ph* dipole strength was concentrated
driven by low-lying isoscalar L=1 modes, transfered momentum $q \approx 0.6$/fm
mostly isoscalar toroidal models (+ few isovector toroidal strength)