Currents in nuclear density functional phenomenology

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Outline

The nuclear many-body problem: from QCD to mean field

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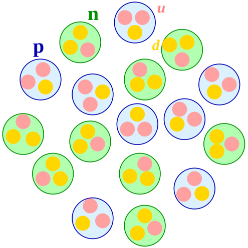

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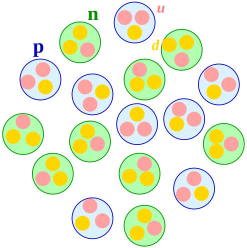

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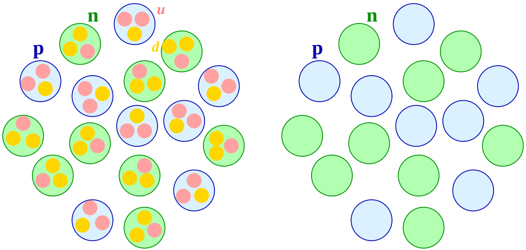

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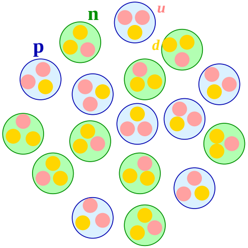

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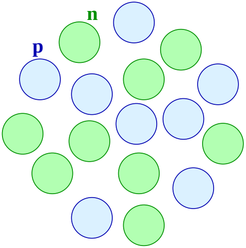

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quality $E \approx 10\%$

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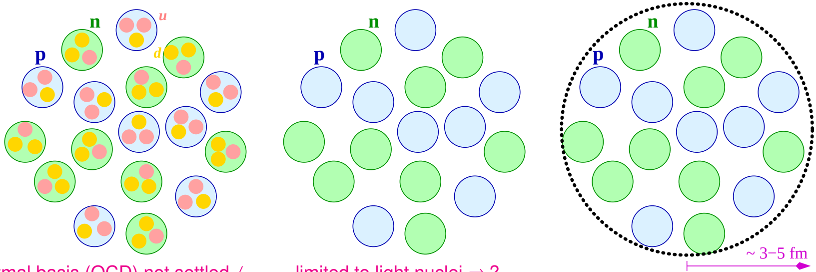

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- common binding potential ≡ mean field

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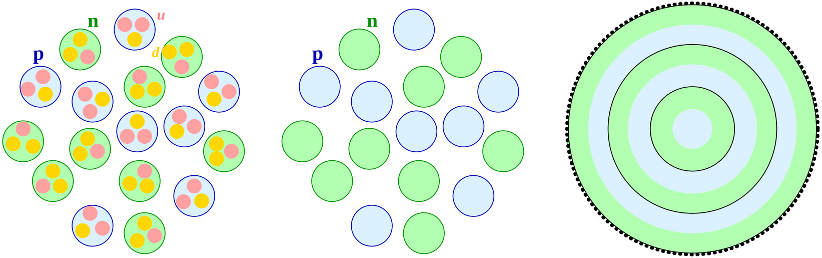

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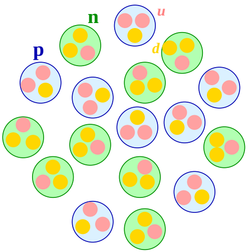

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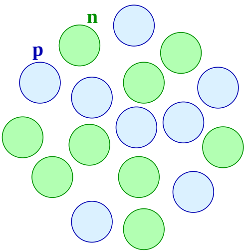

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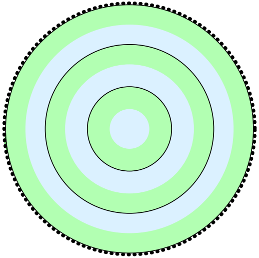

pure “ab initio” not reliable $\lightning$
empirical “ab initio” ?
$\Longrightarrow$ direct empirical fit !
functional form “ab initio”

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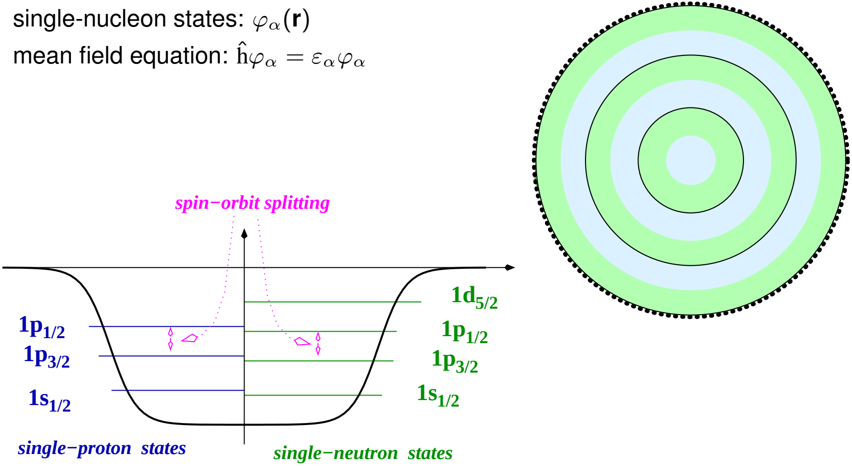
- ignore quark sub-structure $\Longrightarrow$ two-nucleon interactions V_{NN} ??
- common binding potential $\equiv$ mean field
- single nucleon orbit does not resolve details $\Longrightarrow$ “sees” mainly mean field
  $\Longrightarrow$ effective mean-field theory ($\equiv$ DFT), empirically adjusted

Nuclear shell structure

- independent-Fermion state: $\Phi(\mathbf{r}_1 ... \mathbf{r}_N) = \mathcal{A}\{\varphi_1(\mathbf{r}_1)...\varphi_N(\mathbf{r}_N)\}$
- single-nucleon states: $\varphi_\alpha(\mathbf{r})$
- mean field equation: $\hat{\mathrm{h}}\varphi_\alpha = \varepsilon_\alpha \varphi_\alpha$



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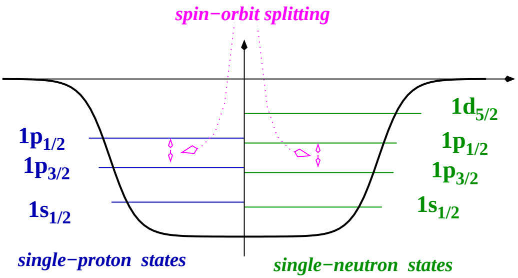
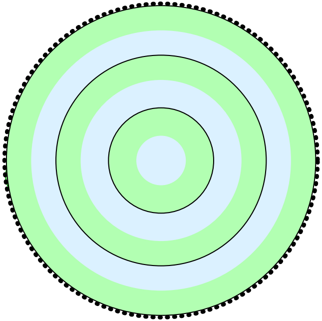
- single-nucleon states: $\varphi_\alpha(\mathbf{r})$
- mean field equation: $\hat{\mathrm{h}}\varphi_\alpha = \varepsilon_\alpha \varphi_\alpha$
- energy-density functional E: $\hat{\mathrm{h}} = \dfrac{1}{\varphi_\alpha} \dfrac{\delta E}{\delta \varphi_\alpha^*}$





Nuclear density functional in the non-relativistic domain

The basic densities and currents

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$$\Phi = \mathcal{A}\{\varphi_1 ... \varphi_N\} \quad \longrightarrow \quad \text{BCS: } |\Phi\rangle = \prod \left(u_\alpha + v_\alpha \hat{a}^\dagger_\alpha \hat{a}^\dagger_{-\alpha} \right) |0\rangle \;, \quad w_\alpha = \left| v_\alpha^2 \right| = \text{occup.}$$

$$\hat{\varrho}_q(\mathbf{r},\mathbf{r}') = \sum_{\alpha \in q} w_\alpha \varphi_\alpha(\mathbf{r}) \varphi^\dagger_\alpha(\mathbf{r}')$$ 1-body density matrix

$$\rho_q(\mathbf{r}) = \mathrm{tr}\{\hat{\varrho}_q(\mathbf{r},\mathbf{r})\} = \sum_{\alpha \in q} w_\alpha \left|\varphi_\alpha(\mathbf{r})\right|^2$$ local density

$$\tau_q(\mathbf{r}) = \mathrm{tr}\{\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{r}'} \hat{\varrho}_q(\mathbf{r},\mathbf{r})\} = \sum_{\alpha \in q} w_\alpha \left|\nabla \varphi(\mathbf{r})\right|^2,$$ kinetic density

$$\mathbf{J}_q(\mathbf{r}) = \frac{1}{\mathrm{i}} \mathrm{tr}\{\nabla_{\mathbf{r}} \times \hat{\sigma} \hat{\varrho}_q(\mathbf{r},\mathbf{r})\} = \frac{1}{\mathrm{i}} \sum_{\alpha \in q} w_\alpha \, \varphi^+_\alpha(\mathbf{r}) \nabla \times \hat{\sigma} \varphi_\alpha(\mathbf{r})$$ spin-orbit density

$$\mathbf{j}_q(\mathbf{r}) = \Im\{\mathrm{tr}\{\nabla_{\mathbf{r}} \hat{\varrho}_q(\mathbf{r},\mathbf{r})\}\} = \sum_{\alpha \in q} w_\alpha \, \Im\left\{\varphi^+_\alpha(\mathbf{r}) \nabla \varphi_\alpha(\mathbf{r})\right\}$$ local current

$$\boldsymbol{\sigma}_q(\mathbf{r}) = \mathrm{tr}\{\hat{\boldsymbol{\sigma}} \hat{\varrho}_q(\mathbf{r},\mathbf{r})\} = \sum_{\alpha \in q} w_\alpha \, \varphi^+_\alpha(\mathbf{r}) \hat{\boldsymbol{\sigma}} \varphi_\alpha(\mathbf{r})$$ spin density

$$\boldsymbol{\tau}_q(\mathbf{r}) = \mathrm{tr}\{\nabla_{\mathbf{r}} \cdot \nabla_{\mathbf{r}'} \hat{\boldsymbol{\sigma}} \hat{\varrho}_q(\mathbf{r},\mathbf{r})\} = \sum_{\alpha \in q} w_\alpha \, \nabla \varphi^+_\alpha(\mathbf{r}) \cdot \nabla \hat{\boldsymbol{\sigma}} \varphi_\alpha(\mathbf{r})$$ kinetic spin density

$$\chi_q(\mathbf{r}) = \sum_{\alpha \in q} u_\alpha v_\alpha \left|\varphi_\alpha(\mathbf{r})\right|^2$$ pair density

recouple: $\rho = \rho_\mathrm{p} + \rho_\mathrm{n} \leftrightarrow$ total density = isoscalar

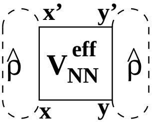
$\tilde{\rho} = \rho_\mathrm{p} - \rho_\mathrm{n} \leftrightarrow$ difference density = isovector

Density-matrix expansion – a low q approximation

Density-matrix expansion – a low *q* approximation

(ignore spin and isospin for simplicity)

$$E_{\text{pot}} = \frac{1}{2}\int d^3x\, d^3x'\, d^3y\, d^3y'\, \varrho(\mathbf{x},\mathbf{x}')\; V_{NN}^{\text{eff}}(\mathbf{x},\mathbf{x}';\mathbf{y},\mathbf{y}';\rho)\; \varrho(\mathbf{y},\mathbf{y}') \;\equiv$$



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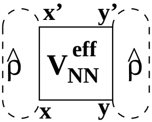

V_{NN}^{eff} well localized $\Longrightarrow$ expand ϱ in orders $(\mathbf{x}-\mathbf{x}')^n$ around $\bar{\mathbf{x}} = (\mathbf{x}+\mathbf{x}')/2$:

$$\varrho(\mathbf{x},\mathbf{x}') \approx \rho(\bar{\mathbf{x}}) + \mathrm{i}(\mathbf{x}-\mathbf{x}')\cdot j(\bar{\mathbf{x}}) + \frac{1}{2}(\mathbf{x}-\mathbf{x}')^2\left(\tau - \frac{1}{4}\Delta\rho\right)$$

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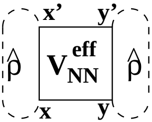

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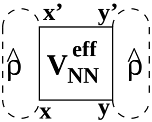

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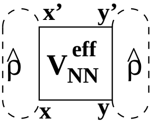

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$f_i \stackrel{?}{=} f_i(\rho) \Longrightarrow$ simple model for density dependence: ρ only in f_0 & only ρ^α

$\Longrightarrow \quad f_0 = B_0 + B_3\rho^\alpha\,,\ f_1 = B_1\,,\ f_2 = \frac{1}{2}B_2\,,\ f_4 = B_4 \quad \Longrightarrow$

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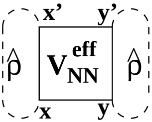

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finally add the same terms for isovector densities $\tilde{\rho}$, $\tilde{\tau}$, $\tilde{\mathbf{j}}$, $\tilde{\mathbf{J}}$, $\tilde{\boldsymbol{\sigma}}$, $\tilde{\tau}$

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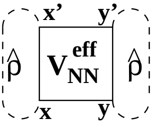

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$\boxed{B_i,\ \alpha}$: in principle derived from $V_{NN}^{\rm eff}$ – in practice free parameters, adjusted to data

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The Skyrme functional

The Skyrme functional (only time even) and physical impact of terms

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

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

kinetic energy

Coulomb en. (exchange = Slater appr.)

$$\frac{\langle\hat{\mathbf{P}}^2_{\mathrm{cm}}\rangle}{2m_N A}$$

center-of-mass

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kinetic energy

$$\frac{\langle \hat{\mathbf{P}}^2_{\rm cm}\rangle}{2m_N A}$$ center-of-mass

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

$\rho_{\rm pair} = \infty \equiv$ volume

$\rho_{\rm pair} = \rho_{\rm equi} \equiv$ surface

The Skyrme functional (only time even) and physical impact of terms

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

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

kinetic energy

$$\frac{\langle \hat{\mathbf{P}}^2_{\text{cm}} \rangle}{2m_N A}$$ center-of-mass

Coulomb en. (exchange = Slater appr.)

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

pairing functional

$\rho_{\text{pair}} = \infty \equiv$ volume

$\rho_{\text{pair}} = \rho_{\text{equi}} \equiv$ surface

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

isoscalar *isovector*

The Skyrme functional (only time even) and physical impact of terms

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

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+ & \frac{1}{2}B_2 & (\nabla\rho)^2 & + & \frac{1}{2}B_2' & (\nabla\tilde{\rho})^2 \\
+ & \frac{1}{2}B_4 & \rho\nabla\mathbf{J} & + & \frac{1}{2}B_4' & \tilde{\rho}\nabla\tilde{\mathbf{J}} \\
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	$\frac{1}{2}B_0$	ρ^2	$+$	$\frac{1}{2}B_0'$	$\tilde{\rho}^2$	}	bulk equil.: E/A, $\rho_{\rm equi}$; incompress.: K
$+$	$\frac{1}{2}B_3$	$\rho^{2+\alpha}$	$+$	$\frac{1}{2}B_3'$	$\tilde{\rho}^2\rho^\alpha$		symmetry energy: $a_{\rm sym}$ and slope $\partial_\rho a_{\rm sym}$
$+$	$\frac{1}{2}B_2$	$(\nabla\rho)^2$	$+$	$\frac{1}{2}B_2'$	$(\nabla\tilde{\rho})^2$		surface en.: $a_{\rm surf}$, surface symm.: $a_{\rm surf,sym}$,
$+$	$\frac{1}{2}B_4$	$\rho\nabla\mathbf{J}$	$+$	$\frac{1}{2}B_4'$	$\tilde{\rho}\nabla\tilde{\mathbf{J}}$		spin-orbit (shell effect, finite nuclei)
$+$	B_1	$\rho\tau$	$+$	B_1'	$\tilde{\rho}\tilde{\tau}$		effective mass: m^*, sum rule enhanc. κ
	isoscalar			*isovector*			*associated bulk properties* *(nuclear matter)*

Observables from mean-field models

Observables from mean-field models

basic nuclear bulk observables:

binding energy E_B , **even-odd staggering** $\Delta_p^{(3)}, \Delta_n^{(3)}$
charge: r.m.s. r_c, **diffr.** R_c, **surface thickn.** σ_c,
spin-orbit splittings $\Delta\varepsilon_\mathrm{ls} = \varepsilon_{l-1/2,l} - \varepsilon_{l+1/2,l}$

} used for calibration in selection of semi-magic nuclei by means of χ^2 fits

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response properties of finite nuclei:

dipole polarizability α_D	constrained mean-field
dipole strengths, giant reson.	TDDFT, small amplitude
fusion, fission, surface vibrations	TDDFT, large amplitude

} probes applications

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} probes applications

$\Updownarrow$ nuclear matter properties to guide calibration of response properties

response properties of nuclear matter ($\leftrightarrow$ pseudo-observable used for characterization):

isoscalar static: **incompressibilty** K, isoscalar dynamic: **effective mass** m^*/m
isovector static: **symmetry energy** a_sym, isovector dynamic: **isovector sum rule** κ

a_sym, m^*/m, κ only loosely determined by g.s. fit $\longleftrightarrow$ check dynamics

Hierarchy of importance for Skyrme functional

Hierarchy of importance for Skyrme functional - 1. volume only (LDA)

$$E = E_{kin} + \int d^3r\, \mathcal{E}(\rho, \tau_{kin}, \vec{J}_{ls}, \tilde{\rho}, \tilde{\tau}_{kin}, \tilde{\vec{J}}_{ls}) + E_C + E_{pair} + E_{cm}$$

volume

two−body: $B_0\, \rho^2 \quad + \quad B_0'\, \tilde{\rho}^2$

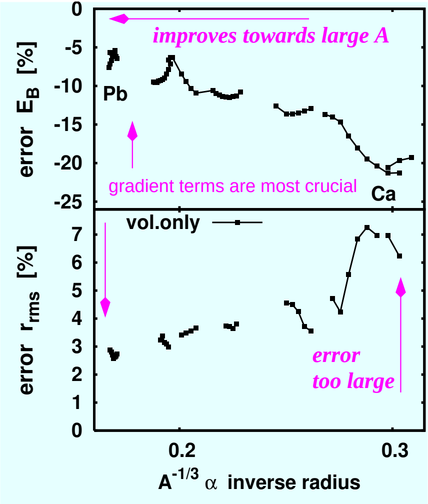
density dep.: $B_3\, \rho^{2+\alpha} \quad + \quad B_3'\, \tilde{\rho}^2 \rho^\alpha$

purely density dependent functional

equivalent to LDA for electronic systems

suffices for perfect description of homogeneous nuclear matter

isoscalar	*isovector*
T=0	*T=1*
$\rho = \rho_p + \rho_n$	$\tilde{\rho} = \rho_p - \rho_n$



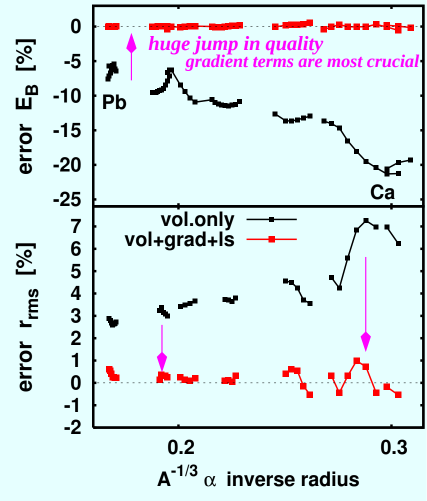
Hierarchy of importance for Skyrme functional - 2. + surface & ls

$$E = E_{kin} + \int d^3r\, \mathcal{E}(\rho, \tau_{kin}, \mathcal{J}_{ls}, \tilde{\rho}, \tilde{\tau}_{kin}, \tilde{\mathcal{J}}_{ls}) + E_C + E_{pair} + E_{cm}$$

volume

two−body	$B_0\rho^2$	$+\ B_0'\tilde{\rho}^2$
density dep.	$B_3\rho^{2+\alpha}$	$+\ B_3'\tilde{\rho}^2\rho^\alpha$
spin −orbit	$B_4\rho\mathcal{J}_{ls}$	
gradient	$B_2(\nabla\rho)^2$	

surf.

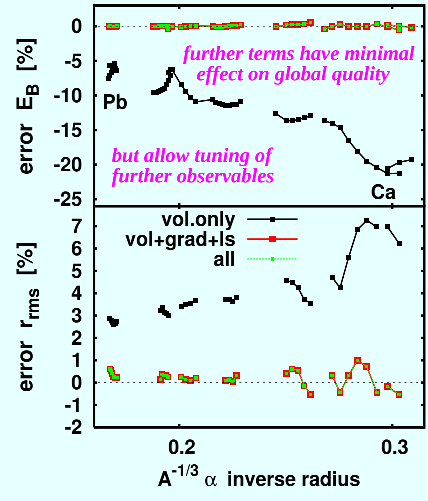


isoscalar	*isovector*
T=0	*T=1*
$\rho = \rho_p + \rho_n$	$\tilde{\rho} = \rho_p - \rho_n$

Hierarchy of importance for Skyrme functional - 3. all terms

$$E = E_{kin} + \int d^3r\, \mathcal{E}(\rho, \tau_{kin}, J_{ls}, \tilde{\rho}, \tilde{\tau}_{kin}, \tilde{J}_{ls}) + E_C + E_{pair} + E_{cm}$$

volume	two−body	$B_0\rho^2$	$+\ B_0'\tilde{\rho}^2$
	density dep.	$B_3\rho^{2+\alpha}$	$+\ B_3'\tilde{\rho}^2\rho^\alpha$
surf.	spin −orbit	$B_4\rho J_{ls}$	$+\ B_4'(\tilde{\rho}\tilde{J}_{ls})$
	gradient	$B_2(\nabla\rho)^2$	$+\ B_2'(\nabla\tilde{\rho})^2$
	kinetic	$B_1\rho\tau_{kin}$	$+\ B_1'\tilde{\rho}\tilde{\tau}_{kin}$
		isoscalar	*isovector*
		T=0	*T=1*
		$\rho = \rho_p + \rho_n$	$\tilde{\rho} = \rho_p - \rho_n$

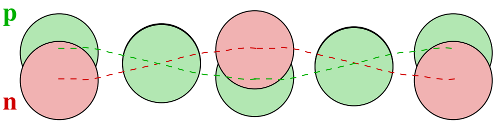


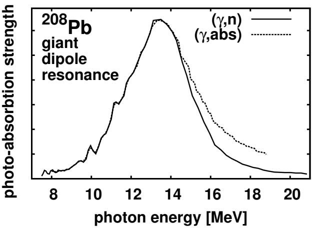
Dynamical observables I: Resonance excitations

Resonance excitations

Nuclei: giant dipole resonance

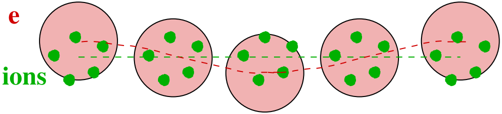
collective dipole mode (Goldhaber–Teller)
proton c.m. ↔ neutron c.m.

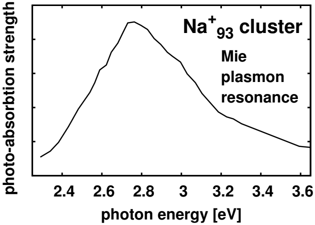




Clusters: Mie plasmon reson.

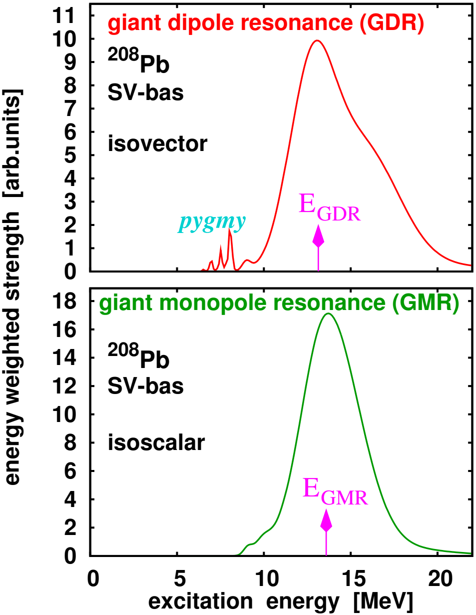
collective dipole mode
electron cloud ↔ ionic background





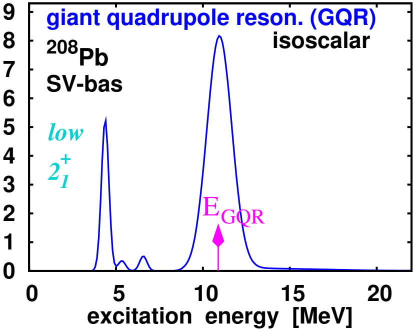
- dipole ⟷ photo-reactions
- Mie plasmon = doorway for laser excit.
- L=0, L=2 reson. ↔ e^-, p, α scattering
- dominant resonance peak
- damping (width) ↔ coupling to 1*ph* (Landau damping/fragmentation)

Collective resonance excitations (example ^{208}Pb)

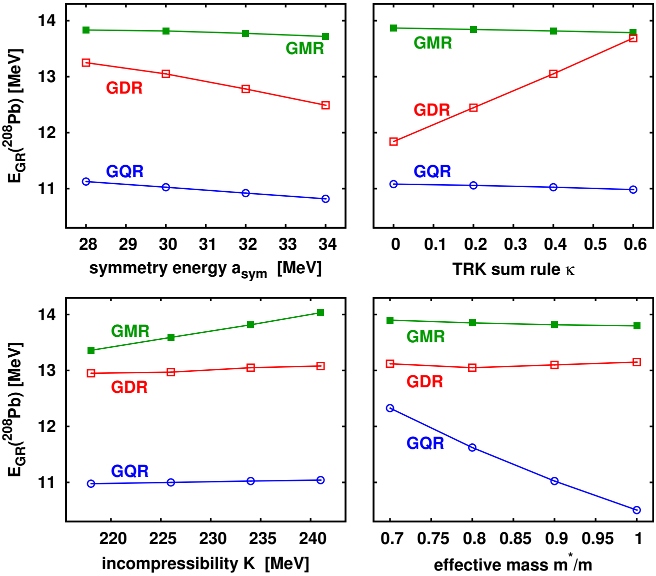


marked resonance peaks
in the region E ~ 12 MeV
well characterizeable by
one resonance energy

width: Landau fragmentation
escape, 2ph collisions



Systematic variation of Skyrme forces



each bulk property is sensitive preferably to one of the 3 modes:

K	↔	*GMR*
m/m*	↔	*GQR*
a_{sym}, κ	↔	*GDR*

and there is some flexibility in the choice of the bulk properties

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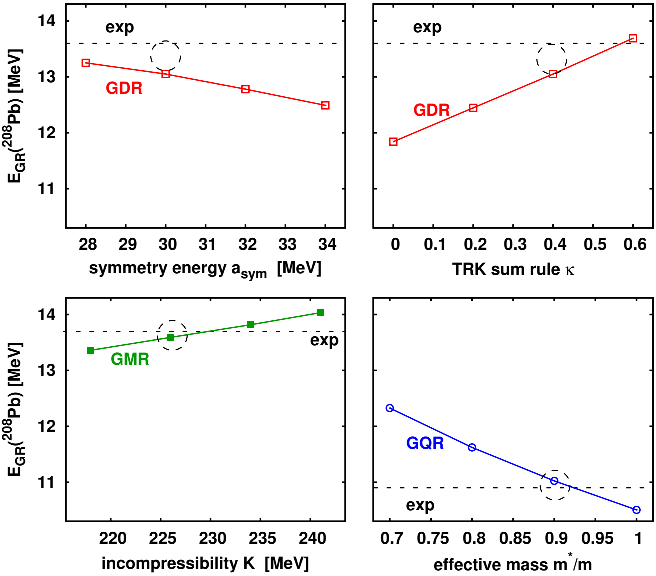

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and there is some flexibility in the choice of the bulk properties

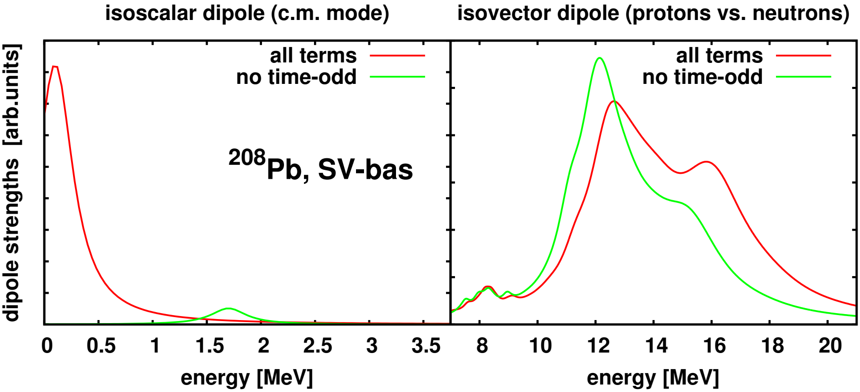
⟹

use this freedom to tune resonances (↔ fix bulk prop.)

Dynamical observables II: Importance of j^2 terms

Importance of $\mathbf{j}^2$ (time-odd) terms

Test case: Dipole excitation spectra in ^{208}Pb - with and without time-odd terms



$\mathbf{j}^2$-terms are crucial for $E_{\mathrm{cm}} = 0$
(Galilean invariance)

$\mathbf{j}^2$-terms are important in general

Dynamical observables III: Fission

Coulomb instability – shell stabilization in nuclear fission

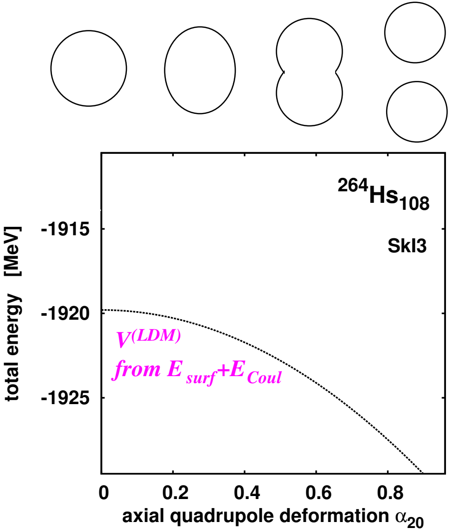
Global estimate of stability for ^{264}Hs:

Coulomb energy E_{Coulomb} repulsive
$\Longrightarrow$ drives system apart = fission

Surface energy E_{surf} attractive
binds and drives to spherical shape

$E_{\mathrm{Coulomb}}(^{264}\mathrm{Hs}) > E_{\mathrm{surf}}(^{264}\mathrm{Hs})$
$\Rightarrow$ ^{264}Hs should explode immediately

potential energy surface along fission path



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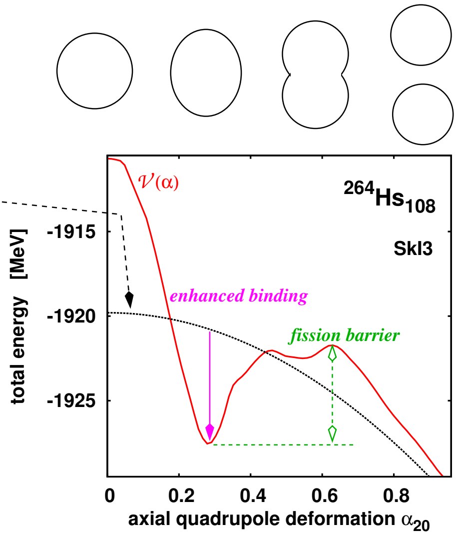
Microscopic picture (mean field):
shell structure adds energy correction
which varies along path
$\Longrightarrow$ deformation energy surface $\mathcal{V}(\alpha)$
has binding pocket and fission barrier

potential energy surface along fission path



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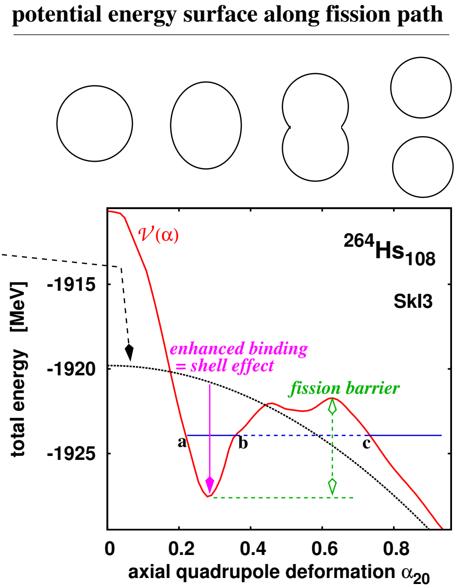
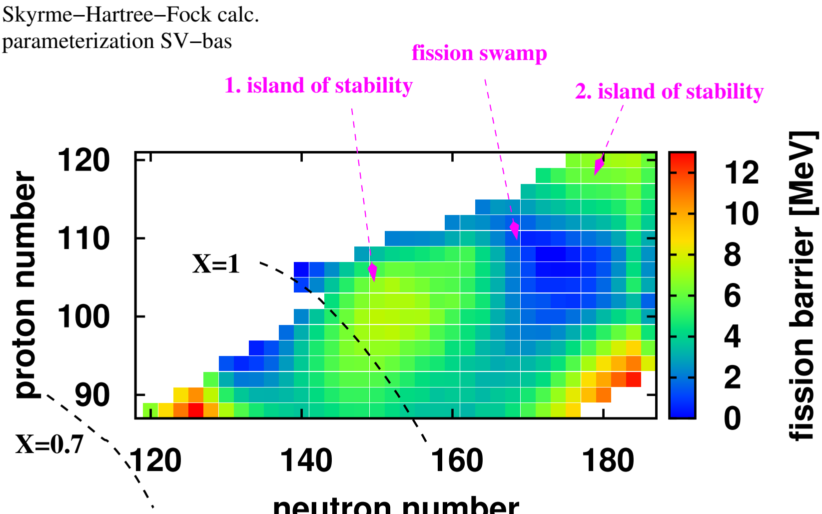
Calculational scheme:
nuclear fission = Q.M. tunneling $b \longrightarrow c$
theory: fully microscopic computation of
- potential $\mathcal{V}(\alpha)$,
- mass $\mathcal{M}(\alpha)$,
- quantum corrections

$\rightarrow$ use in WKB for fission life time τ_{fiss}

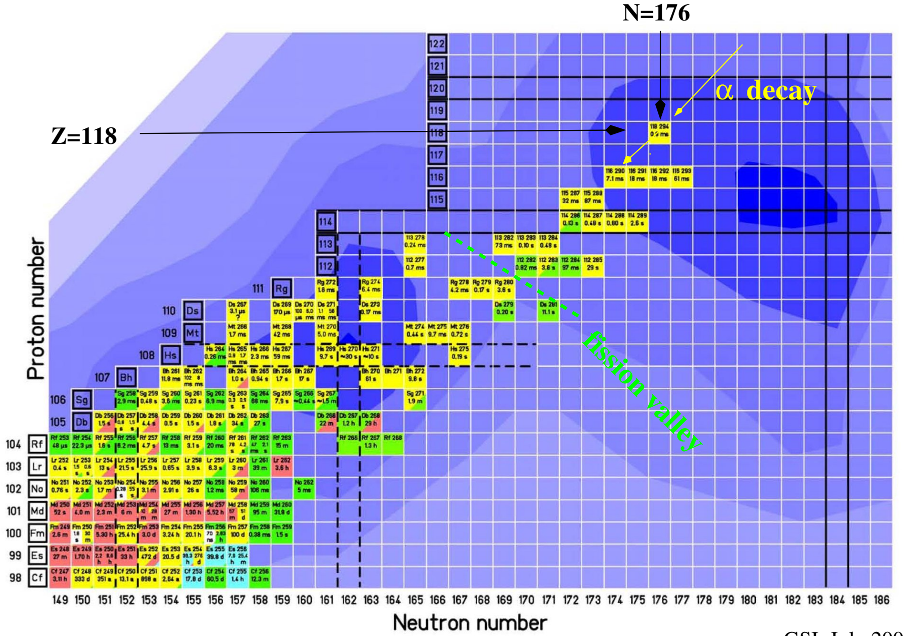


Coulomb instability – systematics of nuclear fission barriers



- nuclei show Coulomb instability
- but with islands of shell stabilization $\Longrightarrow$ super-heavy elements (SHE)

The chart of nuclear isotopes in the realm of heavy elements



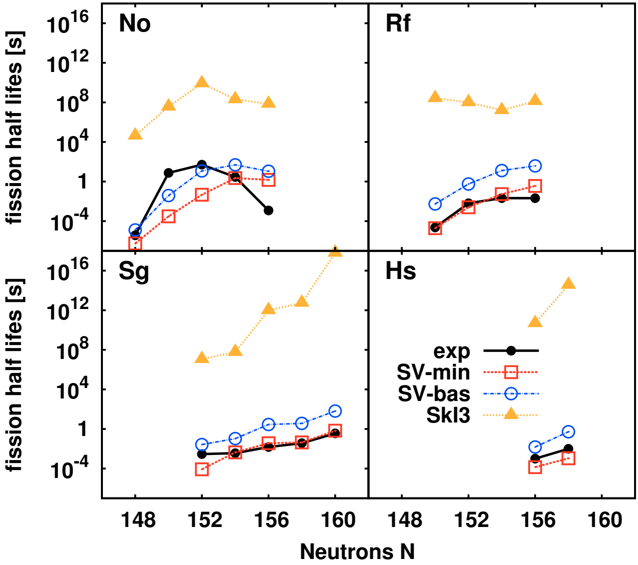
GSI, July 2009

Test fission lifetimes for transactinides

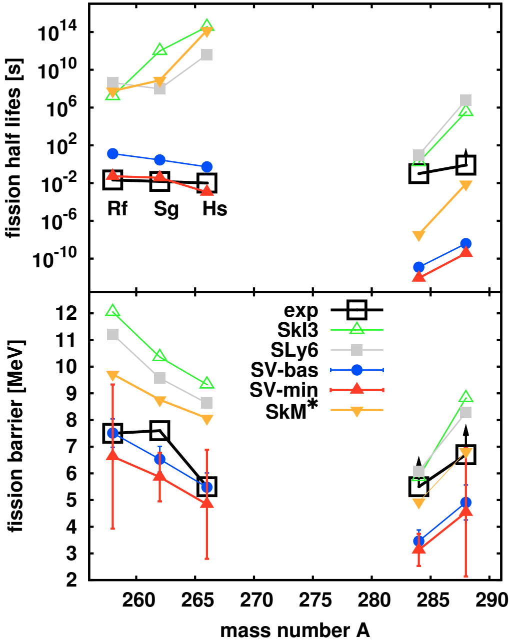
predictions vary sizeably

τ_{fiss} depends on m^*/m

$m^*/m = 0.9 - 1$
$\Rightarrow$ reasonable results



Test fission lifetimes for SHE



unresolved trend:

forces which perform very well for $Z \approx 100$

underestimate τ_{fiss} for $Z \approx 114$

and vice versa

Summary

- Skyrme energy functional: form deduced formally (low q expansion)
  $\mathbf{j}$ combined in $\rho\tau - \mathbf{j}^2$ for Galilean invariance
  $\mathbf{j}$ terms related to effective mass $\neq 1$
  parameters optimized empirically (g.s. nuclei)

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- terms in ρ only $\Longrightarrow$ insufficient
  & $\nabla\rho$& spin-orbit $\Longrightarrow$ sufficiently high precision for g.s.
  & terms in τ,$\mathbf{j}$ $\Longrightarrow$ higher precision for g.s., tuning dynamical props.

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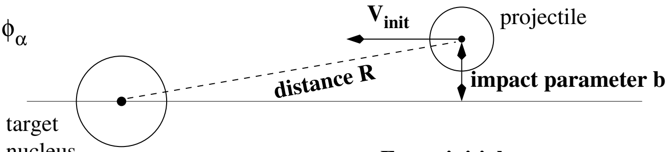
- fit to g.s. properties — some uncertainty in extrapolations
  tune further observables — (surface vibrations, giant resonances, fission, ...)
  $\Longrightarrow$ more reliablility in extrapolations
  exploit, e.g., in astro-physics (super-nova)

Appendix: Dynamical observable IV – fusion

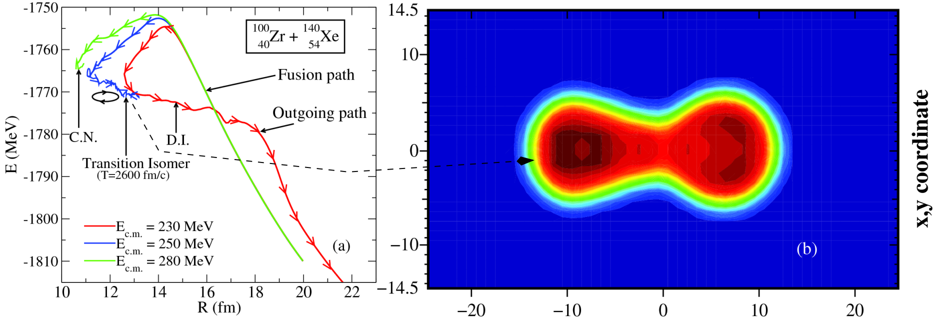
Microscopic simulation (TDHF) of heavy-ion collision – ${}^{100}_{40}$Zr+${}^{140}_{54}$Xe

$$i\partial_t \phi_\alpha = h_{mf}\, \phi_\alpha$$



$v_{init} \Rightarrow E_{cm}$ = initial c.m. energy

potential energy along fusion path **shape of compound system in entrance channel**

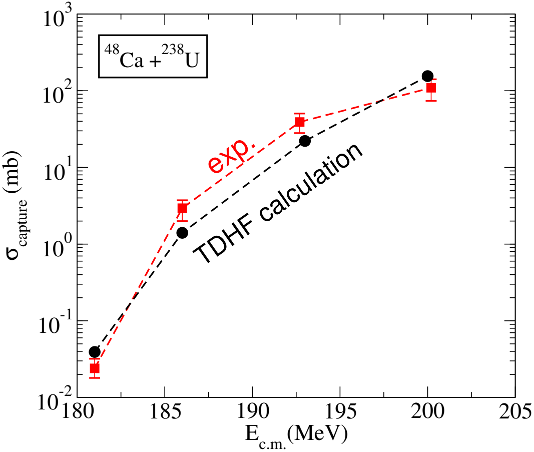


distance between nuclei **z coordinate**

Heavy-ion collisions – fusion cross section for $^{48}Ca+^{208}Pb$

Skyrme–TDHF calculation:

- determine bunch of fusion paths for a couple of impact parameters b
- evaluate collective potential from the paths
- compute collective fusion dynamics in these pots.
- integrate fusion probabil. over impact parameters



Skyrme–TDHF yields a very good description