Density functional methods: from nuclei and nanosystems to astrophysics

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Helmholtz International School

Nuclear Theory and Astrophysical Applications

Dubna, August 7-17, 2007

Content:

Lecture 1:

- density functional theory
- nuclear functional with Skyrme forces:
  - structure
  - t-odd densities
  - fitting procedure, variety of forces

Lecture 2:

- time-dependent version (TD-DFT)
- application of Skyrme functional: nuclei, astrophysics
- Kohn-Sham functional for electronic systems
- nuclear Skyrme functional vs electronic KS functional

Problem solving seminar:

Dipole modes (E1, scissors M1) in various systems:
nuclei, atomic clusters, quantum dots, Bose-Einstein condensate

Density functional theory (1): phylosophy

Basic idea:

To replace a complicated interacting many-body problem:
by much easier effective single-particle problem
which gives the same density of particles $n(\vec{r},t)$

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \qquad \hat{H}(\vec{r}_1,\ldots,\vec{r}_A,t) = \sum_i \frac{\hbar^2}{2m}\nabla_j^2 + \sum_{i>j} V_{ij} + \sum_{i>j>k} V_{ijk} + \ldots$$

$\Psi(\vec{r}_1,\ldots,\vec{r}_A,t)$ **- many-body w. f.**

the same density

$$\rho(\vec{r},t)$$

$$i\hbar\frac{\partial}{\partial t}\phi_j = \hat{h}\phi_j, \qquad \hat{h}[\rho(\vec{r},t)] = \hat{h}_0[\rho_0(\vec{r})] + \hat{h}_{res}[\rho(\vec{r},t)]$$

$$\rho(\vec{r},t) = \sum_j |\phi_j(\vec{r},t)|^2$$

$\phi_j(\vec{r},t)$ **- single-particle orbital**

Does exist any universal scheme for construction of
- static mean-field hamiltonian $h_0[\rho_0]$
- dynamical response hamiltonian $h_{res}[\rho(t)]$**?**
Can this scheme take into account correlations ?

YES!
This is Density Functional Theory

(not HF / TDHF)

Density functional theory (2): advantages

- **Self-consistent:** $h_0[\rho(\vec{r})]$ **and** $h_{res}[\rho(\vec{r},t)]$ **are derived from one and the same source (initial functional)**

$$E[J_\alpha] \to h_0[J_\alpha]\phi_i = \sum_\alpha \frac{\delta E}{\delta J_\alpha}\frac{\delta J_\alpha}{\delta \phi_i^\dagger} = \sum_\alpha \frac{\delta E}{\delta J_\alpha}\hat{J}_\alpha \phi_i$$

$$h_{res}[J_\alpha(t)] = \sum_{\alpha'} \frac{\delta h_0}{\delta J_{\alpha'}}\delta J_{\alpha'}(t) = \sum_{\alpha,\alpha'} \frac{\delta^2 E}{\delta J_{\alpha'}\delta J_\alpha}\delta J_{\alpha'}(t)\hat{J}_\alpha$$

$$\rho(\vec{r},t) = \rho_0(\vec{r}) + \delta\rho(\vec{r},t) \qquad E[\rho] = E[\rho_0] + \underbrace{\frac{\delta E}{\delta \rho}|_{\rho_0}}_{h_0}\delta\rho(t) + \underbrace{\frac{\delta^2 E}{\delta\rho\delta\rho'}|_{\rho_0}}_{h_{res}}\delta\rho(t)\delta\rho'(t) + \ldots$$

- **Simple, not time consuming, realistic results**
- **Universal: one of the basic methods of modern theoretical physics:**
  - **atomic nuclei,**
  - **atomic clusters,**
  - **atoms, molecules,**
  - **various nanosystems,**
  - **quantum transport,**
  - **. . . . .**

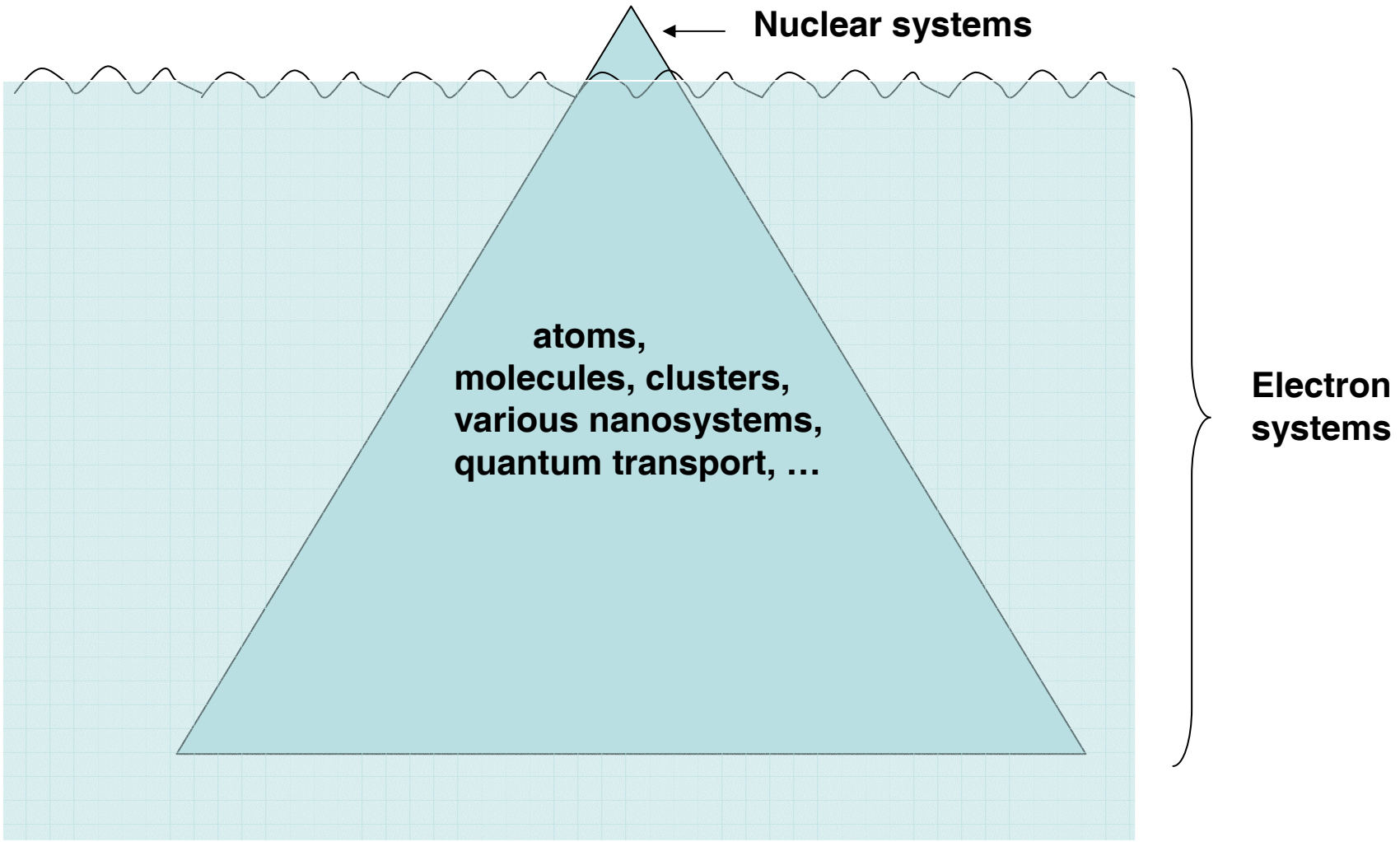
Idea of density functionals is quite old:
e.g. Thomas-Fermi functional (1928)

However, real DFT advent was much later:

- **Skyrme functional for nuclear systems** — T.H.R. Skyrme, 1956; D. Vauterin and D.M. Brink, 1972
- **Kohn-Sham functional for electron systems** — P. Hohenberg and W. Kohn, 1964; W. Kohn and L.J. Sham, 1965

This is because of:
- **nucleons: simple systems, complex forces,**
- **electrons: complex systems, simple forces**

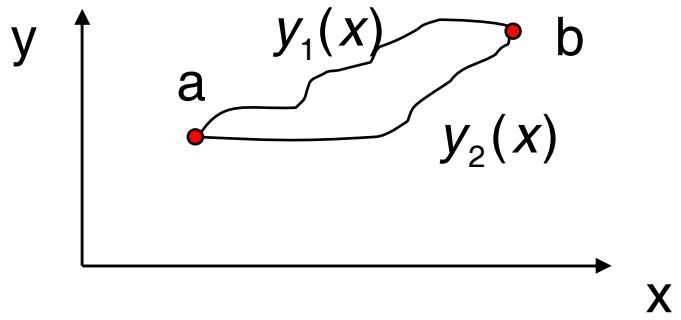
DFT iceberg



Morality: even working only with nuclei, we should pay attention to DFT in general and its last developments for electronic systems (Kohn-Sham functional)

(lecture of Jolos, second part of my lecture)

Functional: simple example



$$dl^2 = dx^2 + dy^2 = dx^2 + (\frac{dy}{dx}dx)^2 = dx^2(1 + (\frac{dy}{dx})^2)$$

$$\Phi[y(x)] = \int_a^b dl = \int_a^b dx\sqrt{1 + (\frac{dy}{dx})^2}$$

function y(x): x $\longrightarrow$ y

functional $\Phi(y)$ y(x) $\longrightarrow$ Φ ⟸ **C - number**

DFT: $E(\rho)$ ⟵ **Energy of the system as a functional of the particle density**

Main methods in nuclear structure physics:

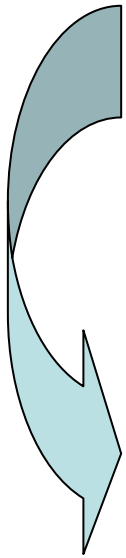
Shell model → (+) Correlations!
(-) small s-p basis, for light and medium nuclei

Relativistic model → In terms of mesons
Correct treatment of spin-orbit. Int.

Skyrme forces → Contact (zero-range) interaction.
Simple treatment.

Gogny forces → Finite-range interaction

} DFT



Universal: all nuclear chart, nuclear and neutron matter,
exotic nuclei (superheavy, drip-line, …)

Skyrme functional: basic points

$$\hat{H}(\vec{r}_1,\ldots,\vec{r}_A,t)=\sum_i\frac{\hbar^2}{2m}\nabla_j^2+\sum_{i>j}V_{ij}+\sum_{i>j>k}V_{ijk}+\ldots$$

$$V_{12}=t\delta(\vec{r}_1-\vec{r}_2),\qquad V_{123}=t_3\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3)$$

$$\left.\begin{aligned}V_{12}&=t_0(1+x_0P_\sigma)\delta(\vec{r}\,')\\&+\frac{1}{2}t_1(1+x_1P_\sigma)[\vec{k}'^2\,\delta(\vec{r}\,')+\delta(\vec{r}\,')\vec{k}^2]\end{aligned}\right\}\text{ - central term}$$

$$+t_2(1+x_2P_\sigma)\,\vec{k}'\cdot\delta(\vec{r}\,')\vec{k}\qquad\text{- non-local term}$$

$$+\frac{1}{6}t_3(1+x_3P_\sigma)[\rho(\vec{r})]^\alpha\delta(\vec{r}\,')\qquad\text{- density-dependent term}$$

$$+iW\vec{\sigma}\cdot[\vec{k}'\times\delta(\vec{r}\,')\vec{k}]\qquad\text{- spin-orbital term}$$

$$\vec{r}=(\vec{r}_1+\vec{r}_2)/2,\quad \vec{r}\,'=\vec{r}_1-\vec{r}_2\qquad \vec{\sigma}=\vec{\sigma}_1+\vec{\sigma}_2,\quad P_\sigma=(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)/2$$

$$\vec{k}=\vec{\nabla}_1-\vec{\nabla}_2)/2i,\quad \vec{k}'=-(\overleftarrow{\nabla}_1-\overleftarrow{\nabla}_2)/2i$$

Skyrme forces

$$E = \int H(\vec{r})\, d\vec{r}, \qquad H = T + H_{Sk} + H_{Coul}$$

$$H_{Sk}(\rho,\tau,\vec{\Im}) = \frac{b_0}{2}\rho^2 - \frac{b'_0}{2}\sum_q \rho_q^2$$

- central term

$$+\frac{b_3}{2}\rho^{\alpha+2} - \frac{b'_3}{2}\sum_q \rho_q^{\alpha+2}$$

- density-dependent term (from 3-body forces)

$$+b_1\rho\tau - b'_1\sum_q \rho_q\tau_q$$

- non-local term (responsible for m*)

$$-\frac{b_2}{2}\rho\Delta\rho + \frac{b'_2}{2}\sum_q \rho_q\Delta\rho_q$$

- surface term

$$-b_4\rho\vec{\nabla}\cdot\vec{\Im} + b'_4\sum_q \rho_q\vec{\nabla}\cdot\vec{\Im}_q$$

- spin-orbital term

$$-b_5\vec{\Im}^2 + b'_5\sum_q \vec{\Im}_q^2$$

- usually neglected

q=p,n

$$b_0 = t_0(1+\frac{1}{2}x_0)$$

$$b'_0 = t_0(\frac{1}{2}+x_0)$$

...

Time-even densities:

$$\rho(\vec{r}) = \sum_j |\phi_j(\vec{r})|^2$$

$$\tau(\vec{r}) = \sum_j |\vec{\nabla}\phi_j(\vec{r})|^2$$

$$\vec{\Im}(\vec{r}) = -i\sum_j \phi_j^+(\vec{r})\vec{\nabla}\times\vec{\sigma}\phi_j(\vec{r})$$

Isoscalar – isovector Skyrme functional:

Neutron-proton Skyrme functional:

$$H_{Sk}(\rho_p, \rho_n, \tau_p, \tau_n, \ldots)$$

$$\rho_{is} = \frac{1}{2}(\rho_p + \rho_n)$$

$$\rho_{iv} = \frac{1}{2}(\rho_p - \rho_n)$$

Isoscalar – isovector Skyrme functional:

$$H_{Sk}(\rho_{is}, \rho_{iv}, \tau_{is}, \tau_{iv}, \ldots)$$

Skyrme functional: two options

Two alternative TD-DFT Skyrme schemes:

1) from Skyrme two-body forces: only t-even densities

T.H.R. Skyrme, 1956
D. Vauterin, D.M. Brink, 1972

$$\rho, \tau, \vec{J}$$

2) as bilinear form of densities and their first and second derivatives : both t-even and t-odd densities

Y.M. Engel, 1975
J. Dobaczewski, J. Dudek, 1995

$$\rho, \tau, \vec{J}, \vec{\sigma}, \vec{j}, \vec{T}$$

Do we really need in TD-DFT t-odd densities?

Skyrme functional for atomic nuclei

Y.M. Engel et al, NPA 249, 215 (1975).
J. Dobaczewski and J. Dudek, PRC, 52 1827 (1995).

$$E = \int H(\vec{r})\, d\vec{r}, \qquad H = T + H_{Sk} + H_{Coul}$$

$$H_{Sk}(\rho,\tau,\vec{\Im},\vec{j},\vec{s},\vec{T}) = \frac{b_0}{2}\rho^2 - \frac{b_0'}{2}\sum_q \rho_q^2 + \frac{b_3}{2}\rho^{\alpha+2} - \frac{b_3'}{2}\sum_q \rho_q^{\alpha+2}$$
$$+ b_1(\rho\tau - \vec{j}^{\,2}) - b_1'\sum_q(\rho_q\tau_q - \vec{j}_q^{\,2}) - \frac{b_2}{2}\rho\Delta\rho + \frac{b_2'}{2}\sum_q \rho_q\Delta\rho_q$$
$$- b_4(\rho\vec{\nabla}\cdot\vec{\Im} + \vec{s}\cdot(\vec{\nabla}\times\vec{j})) + b_4'\sum_q(\rho_q\vec{\nabla}\cdot\vec{\Im}_q + \vec{s}_q\cdot(\vec{\nabla}\times\vec{j}_q)) + \ldots$$

q=p,n

(+) nucleon dens. $\rho(\vec{r}) = \sum_j |\phi_j(\vec{r})|^2$

(+) kin. en. dens. $\tau(\vec{r}) = \sum_j |\vec{\nabla}\phi_j(\vec{r})|^2$

(+) spin-orb. dens. $\vec{\Im}(\vec{r}) = -i\sum_j \phi_j^+(\vec{r})\vec{\nabla}\times\vec{\sigma}\phi_j(\vec{r})$

Time-even: $\hat{T}\rho\hat{T}^{-1} = \rho$

Contribute both to the ground state and excitations.

(-) current $\vec{j}(\vec{r}) = -\frac{i}{2}\sum_j(\phi_j^+(\vec{r})\vec{\nabla}\phi_j(\vec{r}) - \phi_j(\vec{r})\vec{\nabla}\phi_j^+(\vec{r}))$

(-) spin dens. $\vec{s}(\vec{r}) = -i\sum_j \phi_j^+(\vec{r})\vec{\sigma}\phi_j(\vec{r})$

(-) spin kin. en. dens. $\vec{T}(\vec{r}) = \sum_j \vec{\nabla}\phi_j(\vec{r})\vec{\sigma}\cdot\vec{\nabla}\phi_j(\vec{r})$

Time-odd: $\hat{T}\,\vec{j}\,\hat{T}^{-1} = -\vec{j}$

Contribute only to excitations.

Which densities do we need?

Formal arguments:

Single-particle density matrix:

$$\rho(\vec{r}\sigma,\vec{r}\,'\sigma') = \sum_i \phi_i(\vec{r},\sigma)\phi_i{}^*(\vec{r}\,',\sigma') \qquad \rho(\vec{r},\vec{r}\,') = \sum_\sigma \rho(\vec{r}\sigma,\vec{r}\,'\sigma),$$

$$= \frac{1}{2}[\rho(\vec{r},\vec{r}\,')\delta_{\sigma\sigma'} + \sum_\nu \langle\sigma\,|\,\hat{\sigma}_\nu\,|\,\sigma'\rangle\, s_\nu(\vec{r},\vec{r}\,')] \qquad s_\nu(\vec{r},\vec{r}\,') = \sum_{\sigma\sigma'} \rho(\vec{r}\sigma,\vec{r}\,'\sigma')\langle\sigma'\,|\,\hat{\sigma}_\nu\,|\,\sigma\rangle$$

Other densities are first and second derivatives of basic densities ρ, $\vec{s}$:

$$\rho(\vec{r}) = \rho(\vec{r},\vec{r}) \qquad \vec{s}(\vec{r}) = \vec{s}(\vec{r},\vec{r})$$

basic densities

$$\vec{j}(\vec{r}) = \frac{1}{2i}[(\vec{\nabla}-\vec{\nabla}')\rho(\vec{r},\vec{r}\,')]_{\vec{r}=\vec{r}'} \qquad \vec{\Im}_{\mu\nu}(\vec{r}) = \frac{1}{2i}[(\vec{\nabla}_\mu-\vec{\nabla}_\mu')s_\nu(\vec{r},\vec{r}\,')]_{\vec{r}=\vec{r}'}$$

their momenta (first derivatives)

$$\tau(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\,\rho(\vec{r},\vec{r}\,')]_{\vec{r}=\vec{r}'} \qquad \vec{T}(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\,\vec{s}(\vec{r},\vec{r}\,')]_{\vec{r}=\vec{r}'}$$

their kin. energies (second derivatives)

Functional involves all possible bilinear combinations of the basic densities ρ, $\vec{s}$ and their first and second derivatives.

- **Some kind of gradient expansion (important for non-uniform systems)**
- **Combinations of densities in the functional must:**
  - **a) be time-even,**
  - **b) fulfill local gauge (Galilean) invariance**

Local gauge (Galilean) invariance

Local gauge transformation

$$\Psi' = \exp\{i\sum_{j=1}^{N}\varphi(\vec{r}_j)\}\Psi$$

$\varphi(\vec{r})$ **is real function**

Galilean transformation

$$\varphi(\vec{r}) = \frac{\vec{p}_{boost}\cdot\vec{r}}{\hbar}$$

$$\vec{p}_{boost} = const$$

t-odd densities come only in specific combinations with t-even densities:

$$\rho\tau - \vec{j}^{\,2} \qquad \rho\vec{\nabla}\cdot\vec{\Im} + \vec{s}\cdot(\vec{\nabla}\times\vec{j}) \qquad \vec{s}\cdot\vec{T} - \vec{\Im}^{\,2}$$

← **from Galilean invariance**

Hence no new parameters in the functional!

So Galilean invariance allows to introduce t-odd densities without new parameters!

Functionals without t-odd densities do not hold Galilean invariance!

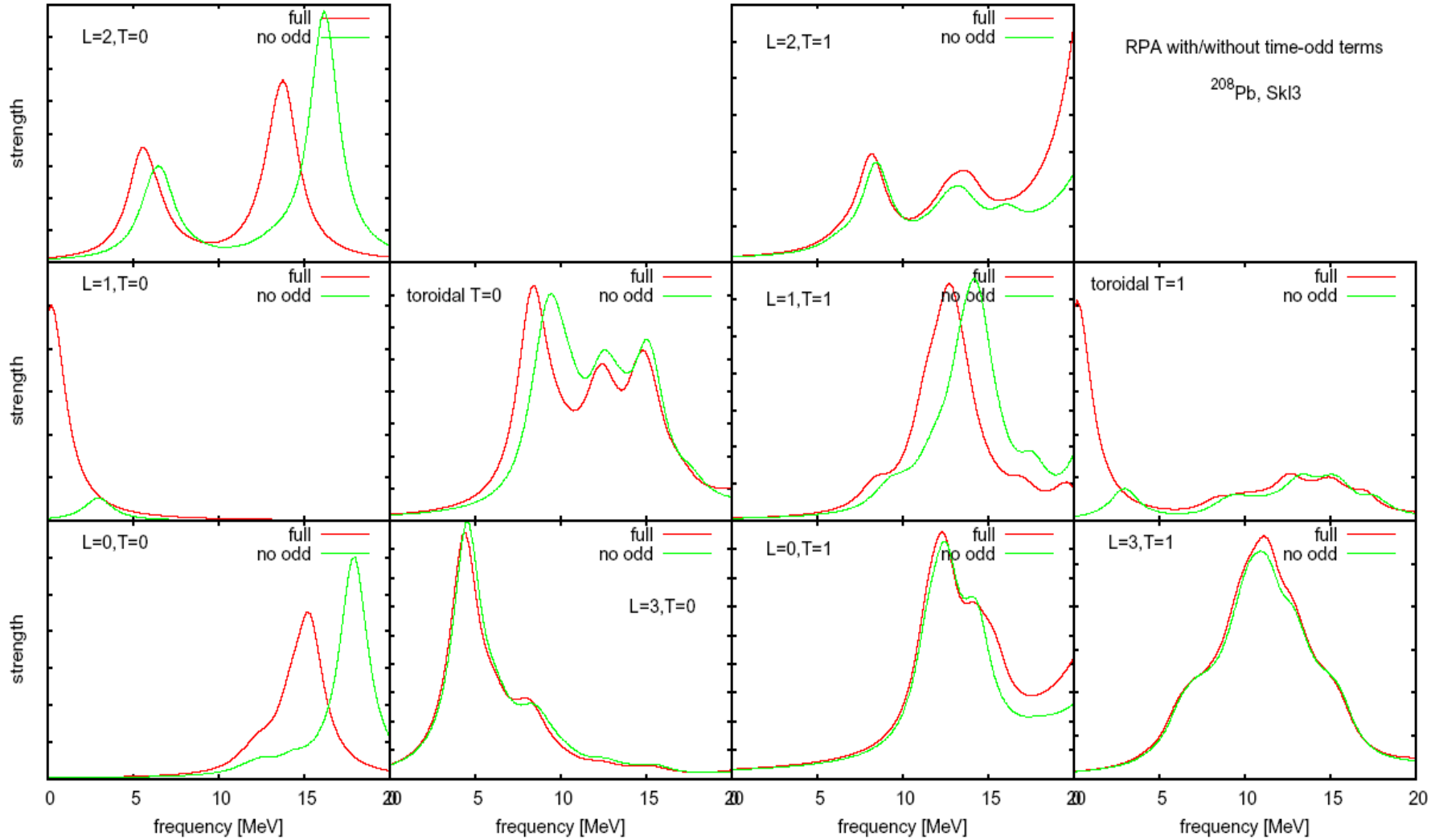
So, we need t-odd densities to :
- **take into account first and second derivatives of the basic densities,**
- **to hold Galilean invariance.**

No new parameters.

⇐ **Strong formal arguments in favor of t-odd densities**

Physical arguments (1):

Influence of T-odd densities on giant resonances (P.-G. Reinhard)



Physical arguments (2):

Some collective modes naturally need t-odd densities:

- Spin M1 mode: $\vec{s}$

-Toroidal E1 mode: $\vec{j}$

- …

DFT formalism: static ground state (1)

$$E[J_\alpha(\vec{r})] = \langle \Psi | H | \Psi \rangle, \qquad \Psi \leftarrow \text{Slater determinant from s-p orbitals } \phi_j(\vec{r})$$

$$J_\alpha(\vec{r}) = < \Psi | \hat{J}_\alpha | \Psi > \in \{\rho(\vec{r}), \tau(\vec{r}), \vec{\Im}(\vec{r})\} \leftarrow \text{Only T-even densities}$$

$$\bar{E} = E[J_\alpha] - \sum_j \varepsilon_j (\phi_j^* \phi_j - 1) \qquad \frac{\delta \bar{E}}{\delta \phi_j^*} = 0$$

$$h_0[J_\alpha]\phi_i = \sum_\alpha \frac{\delta E}{\delta \phi_i^*} = \sum_\alpha \frac{\delta E}{\delta J_\alpha} \frac{\delta J_\alpha}{\delta \phi_i^*} = \sum_\alpha \frac{\delta E}{\delta J_\alpha} \hat{J}_\alpha \phi_i \leftarrow$$

Static mean field hamiltonian for g.s.

(+) nucleon dens. $\rho(\vec{r}) = \sum_j \phi_j^*(\vec{r})\phi_j(\vec{r}) \longrightarrow \hat{\rho}(\vec{r}) = \sum_j \delta(\vec{r} - \vec{r}_j)$

(+) kin. en. dens. $\tau(\vec{r}) = \sum_j \vec{\nabla}\phi_j^*(\vec{r}) \cdot \vec{\nabla}\phi_j(\vec{r}) \longrightarrow \hat{\tau}(\vec{r}) = \sum_j \overleftarrow{\nabla}\delta(\vec{r} - \vec{r}_j)\vec{\nabla}$

(+) spin-orb. dens. $\vec{\Im}(\vec{r}) = -i\sum_j \phi_j^*(\vec{r})\vec{\nabla} \times \vec{\sigma}\phi_j(\vec{r}) \longrightarrow \vec{\Im}(\vec{r}) = -i\sum_j \delta(\vec{r} - \vec{r}_j)\vec{\nabla} \times \vec{\sigma}$

$$h_0^q[J_\alpha(\vec{r})] = \frac{\delta E}{\delta \rho_q} + \overleftarrow{\nabla}\frac{\delta E}{\delta \tau_q}\vec{\nabla} - i\frac{\delta E}{\delta \vec{\Im}_q}\vec{\nabla} \times \vec{\sigma} \qquad \textbf{q=p,n}$$

DFT formalism: static ground state (2)

Schredinger eq.

$$\hat{h}_0[J_\alpha]\phi_j(\vec{r}) = \varepsilon_j \phi_j(\vec{r})$$

- solutions by iterations

$$\phi_j \rightarrow J_\alpha \rightarrow \hat{h}_0[J_\alpha] \rightarrow SE$$

Time-odd densities do not contribute to the g.s. of even-even nuclei

$$\hat{J}^\dagger = \hat{J}, \quad T^{-1}\hat{J}T = \gamma_T^J \hat{J}, \quad \gamma_T^J = \pm 1 \qquad T\,|\,j\rangle = |\,\bar{j}\rangle$$

$$J = \langle \Psi\, \hat{J} \Psi \rangle = \sum_j (\langle j\,|\,\hat{J}\,|\,j\rangle + \langle \bar{j}\,|\hat{J}\,|\,\bar{j}\rangle)$$

$$\langle \bar{j}\,|\,\hat{J}\,|\,\bar{j}\rangle = \langle j\,|\,T\,\hat{J}T^{-1}\,|\,j\rangle^* = \gamma_T^J \langle j\,|\,\hat{J}\,|\,j\rangle^*$$

$$= \gamma_T^J \langle j\,|\,\hat{J}^\dagger\,|\,j\rangle = \gamma_T^J \langle j\,|\,\hat{J}\,|\,j\rangle$$

However, for description of

- g.s. of odd-A and odd-odd nuclei

- nuclear dynamics

we need time-odd densities as well

In fact we use Kohn-Sham procedure though Kohn-Hohenberg theorem was not yet proved for nuclei

Fitting procedure (1)

Skyrme forces: 11 parameters:

$t_0, x_0, t_1, x_1, t_2, x_2, t_3, x_3, t_4, x_4, \alpha$ **or** $b_0, b'_0, b_1, b'_1, b_2, b'_2, b_3, b'_3, b_4, b'_4, \alpha$

- **One can obtain a huge number of different parametrizations**
- **Reasonable fitting strategy is very important**

Nowadays the following sequence of fitting steps is used:

See, e.g. E. Chabanat et al, NPA, 627 710(1997)

- **Symmetric nuclear matter to reproduce**

  ρ_0 - **saturation density**

  e_∞ - **binding energy per nucleon**

  K - **incompressibility**

  m*/m - **isoscalar effective mass**

  } t_0, t_3, α **combination of** t_1, x_1, t_2, x_2

2) Asymmetric nuclear matter to reproduce

a_s - **symmetry energy**

m_1^* / m - **isovector effective mass**

} **Important for exotic drip-line nuclei**

3) Pure neutron matter to reproduce EOS

4) Fine tuning: Binding energies and r.m.s. radii of selected doubly magic nuclei. Spin-orbital splitting of the neutron p-shell in ^{208}Pb

Fitting procedure (2)

As a rule, the fitting is done for:

- **the ground state (isoscalar properties), E0, E2 GR**
- **E1, giant resonance (isovector properties)**

In spite of a generally common fitting strategy, every Skyrme force is usually fitted with a certain bias:

Force	To describe:
SkT6 (1984), SkSC, MSk (2000)	- nuclear masses (MSk: 1719 nuclei) (m*/m = 1.00 - 1.05)
SkM* (1982)	- isoscalar E2 giant resonance, fission barriers (m*/m = 0.79)
SLy6 (1997)	- isovector properties of nuclear matter (m*/m = 0.69)
SkI3 (1995)	- isotope shift of r.m.s. radii in neutron rich Pb region (m*/m = 0.58)

Tables for main Skyrme forces e_∞

Force	ρ_0 [fm^{-3}]	E/A [MeV]	K [MeV]	m_0^*/m	k	m_1^*/m	a_{sym} [MeV]
SkT6	0.161	-15.96	237	1.00	0.00	1.00	30.0
SkM*	0.160	-15.77	217	0.79	0.53	0.65	30.0
SLy6	0.159	-15.92	231	0.69	0.25	0.80	32.0
SkI3	0.158	-15.98	259	0.58	0.25	0.80	34.8

Nuclear matter values:

m_0^*/m - **isoscalar effective mass**

m_1^*/m - **isovector effective mass**

ρ_0 - **saturation density**

k - **sum rule enhancement factor**

$$m_1^*/m = \frac{1}{1+k}$$

E/A - **binding energy per nucleon**

K - **incompressibility**

a_{sym} - **symmetry energy coeff.**

$\rho_0 = 0.16 \pm 0.005$ fm^{-3} $\quad E/A = -16.0 \pm 0.2$ MeV $\quad K = 210 \pm 20$ MeV

Variety of Skyrme parametrizations

We have now

~ 100 different Skyrme forces

and

no one universal!

though only few of them are widely recognized and used:

SkT6, SkM*, SLy4, SLy6, SkP, SGII, SkI3,

Nevertheless there is indeed very urgent problem to construct an Universal Nuclear Energy Density Functional!

New initiative in nuclear theory: UNEDF

www.unedf.org

Supervisor G. F. Bertsch
(University of Washington)

Goal: to build

Universal Nuclear Energy Density Functional (UEDF)

- US Department of energy, December 2006: project UNEDF
- Inside SciDAC (Scientific discovery through Advanced Computing)
- 1st cycle: lattice QCD (2000)
  2nd cycle: UNEDF(2006), 3 million dollars per year for 5 years (2 –nucl. phys, 1- comp.)

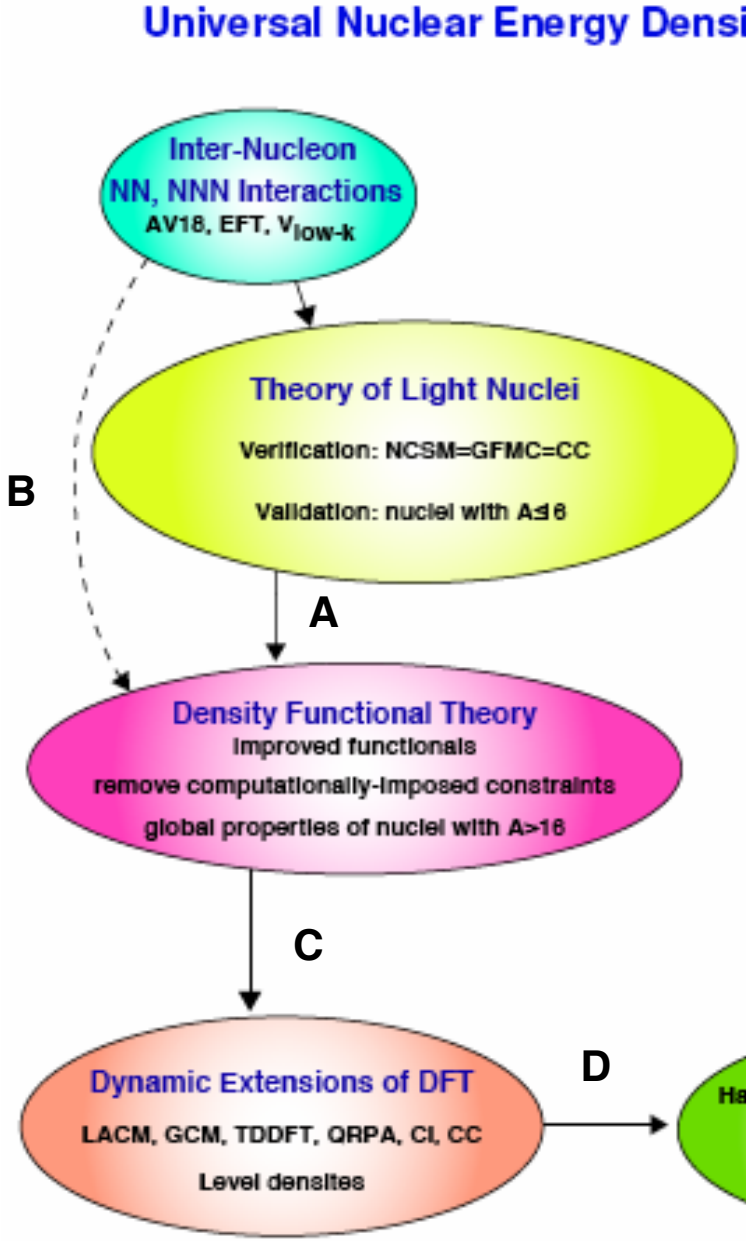
UNEDF:

- 30- 40 researchers from US, Belgium, France, Japan, Poland
- 16 US groups from various universities
- project is opened for researchers from other countries

Motivation:

- building reactors
- great DFT success in condensed matter physics and chemistry
  NP should repeat condensed matter's success.

Microscopic functionals, Skyrme, Gogny, relativistic.



Strategy:

Ab initio theory as a fundamental level.

B: Functionals based directly on the microscop. Hamiltonian.

A: Microscopic calculations for nuclear properties which cannot be determined experimentally.

C: DFT extensions, first of all in dynamics!

D: low-energy nuclear reactions, fission

There has been hardly any systematic study of nuclear properties

↓

need in better codes, parallel processing, …

Thank you for attention!

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Density functional methods: from nuclei and nanosystems to astrophysics

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Lecture II

Helmholtz International School

Nuclear Theory and Astrophysical Applications

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Content:

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- nuclear functional with Skyrme forces:
  - structure
  - t-odd densities
  - fitting procedure, variety of forces

Lecture 2:

- Kohn-Sham functional for electronic systems
- nuclear Skyrme functional vs electronic KS functional
- time-dependent version (TD-DFT)
- application of Skyrme functional:
  - finite nuclei: g.s., dynamics,
  - nuclear matter, astrophysics

Progress in density functional theory (DFT) for electronic systems

- **Hohenberg, Kohn (1964): theorem for non-degenerate ground state**

- **Kohn, Sham (1965): mean field equations for valence electrons**

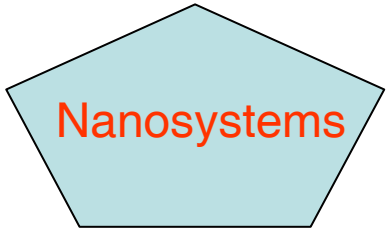
- **Mermin (1965) : theorem for temperature**

- **Gunnarsson, Lundqvist (1976) : xc for spin densities** $\sigma\downarrow$ **and** $\sigma\uparrow$

- **Levy (1979): degenerate ground state**

- **Runge, Gross (1984): time-dependent DFT: TD-DFT**

- **Vignale, Kohn (1996): current TD-DFT**



TD-DFT for electron systems: recent suspects

In

Van Leeuwen, Int. J. Mod. Phys., B15, 1969 92001)
J. Schirmer and A. Dreuw, PRA, 75, 022513 (2007)

the theorem of Runge and Gross was critically reexamined
and stated to be invalid.

Reasons:
- undefined phase factors corrupt RG action integral functionals
- pp- hh-channel was not included. This creates problems for non-local external potentials

This point is still under discussion.

What about t-odd densities in TD-DFT for electron systems?

Can we learn something useful for nuclear physics from electron DFT/TD-DFT?

Kohn-Sham functional for electronic systems:

$$E[\rho_e] = T_{kin} + E_{Coul}[\rho_e] + E_{xc}[\rho_e]$$

$$E_{Coul}[\rho_e] = 1/2 \iint d\vec{r}\, d\vec{r}_1 \frac{(\rho_e(\vec{r},t) - \rho_i(\vec{r}))(\rho_e(\vec{r}_1,t) - \rho_i(r_1))}{|\vec{r} - \vec{r}_1|}$$

- Coulomb energy

(e-i, i-i $\longrightarrow$ V_{ext} **)**

$$E_{xc}[\rho_e] = \int d\vec{r}\ \varepsilon_{xc}[\rho_e(\vec{r},t)]\rho_e(\vec{r},t)$$

- exchange-correlation energy

KS (4): KS equations for electronic mean field

W. Kohn and L.J. Sham, Phys. Rev., 140 (1965) A1133

$$\hat{h}_0(\vec{r})\varphi_j(\vec{r}) = \frac{\delta E[\rho_e]}{\delta \varphi_j^*}\Big|_{\rho_e=\rho_e^0} = \frac{\delta E[\rho_e]}{\delta \rho_e}\Big|_{\rho_e=\rho_e^0} \frac{\delta \rho_e}{\delta \varphi_j^*}$$

Kohn-Sham equations:

$$\hat{h}_0(\vec{r})\varphi_i(\vec{r}) = e_i\varphi_i(\vec{r})$$

$$\hat{h}_0(\vec{r}) = -\frac{\nabla^2}{2} + U_{Coul}(\vec{r}) + U_{xc}(\vec{r})$$

$$U_{Coul}(\vec{r}) = \int d\vec{r}_1 \frac{\rho_e^0(\vec{r}) - \rho_i(\vec{r})}{|\vec{r} - \vec{r}_1|}$$

$$U_{xc}(\vec{r}) = \varepsilon_{xc}[\rho_e^0(\vec{r})] + \rho_e^0(\vec{r})\frac{\delta \varepsilon_{xc}[\rho_e^0(\vec{r})]}{\delta \rho_e^0}$$

$$\rho_e^0(\vec{r}) = \sum_j^{occ} (\varphi_j(\vec{r}))^2$$

- **KSE reduce the correlated many-body problem to a self-consistent mean-field problem of Hartree type**

- **solutions by iterations**

$$\varphi_i \rightarrow \rho_e^0 \rightarrow \hat{h}_0 \rightarrow KSE$$

- **quasi-vanishing U_{Coul} domination of U_{xc}**

- **ionic density**

$$\rho_i(\vec{r}) = \begin{cases} [\frac{4\pi}{3} r_s^3]^{-1}, & r \le R \\ 0, & r > R \end{cases}$$

Why Kohn-Sham and Skyrme functional have so different structure?

Skyrme functional: ⟺ **Kohn-Sham functional:**

- No xc-term,

- Has xc-term,

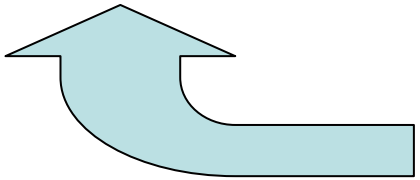
- Form of the basic interaction is unknown, correlations and exchange are put to parameters

- Includes well known basic (Coulomb) interaction, correlations and exchange are introduced as separate corrections to basic interaction

- wide set of densities

$\rho, \tau, J, \sigma, j, \vec{T}$ ⟺

- Mainly the basic electron density ρ_e but, the others can be also introduced.



The current j may be the basic density in TD-DFT if the system is strictly non-uniform!

G. Vignale, W.Kohn, PRL, 77 2037 (1996).

Time-dependent DFT(1)

Time-dependent formulation:

$$E(J_\alpha(\vec{r},t)) = \langle \Psi | H | \Psi \rangle,$$

$$J_\alpha(\vec{r},t) \in \{\rho(\vec{r},t), \vec{j}(\vec{r},t), \ldots\} \qquad J_\alpha(\vec{r},t) = \langle \Psi | \hat{J}_\alpha | \Psi \rangle \quad \leftarrow$$ T-even and T-odd densities

$$J_\alpha(\vec{r},t) = \bar{J}_\alpha(\vec{r}) + \delta J_\alpha(\vec{r},t) \quad \leftarrow$$ Linear regime: small time-dependent perturbation

$$\hat{h}(\vec{r},t) = h_0(\vec{r}) + \delta h_{res}(\vec{r},t) \quad \leftarrow$$ Mean field hamiltonian: static g.s. + time-dependent response

$$= \sum_\alpha \left[\frac{\delta E}{\delta J_\alpha}\right]_{J=\bar{J}} \hat{J}_\alpha(\vec{r}) + \sum_{\alpha\alpha'} \left[\frac{\delta^2 E}{\delta J_\alpha \delta J_{\alpha'}}\right]_{J=\bar{J}} \delta J_\alpha(\vec{r},t)\, \hat{J}_\alpha(\vec{r})$$

$$\delta J_\alpha(t) = \langle \Psi(t) | J_\alpha | \Psi(t) \rangle - \langle 0 | J_\alpha | 0 \rangle \qquad \Psi(t) \leftarrow$$ **Slater determinant from s-p orbitals** $\phi_j(\vec{r},t)$

Calculation scheme:

1) Determination of static orbitals for the g.s.

$$\hat{h}_0(\vec{r})\phi_j(\vec{r}) = \varepsilon_j \phi_j(\vec{r})$$

2) Determination of time evolution of orbitals

$$i\hbar \frac{\partial}{\partial t}\phi_j(\vec{r},t) = \hat{h}(\vec{r},t)\phi_j(\vec{r},t)$$

$$t = 0, \Delta t, 2\Delta t, \ldots$$

TD-DFT formalism (2)

After getting $\phi_j(\vec{r},t)$ **,**

we can determine the density $\rho(\vec{r},t)=\sum_j |\phi_j(\vec{r},t)|^2$

and various oscillating characteristics,
e.g. dipole moment in time domain

$$D(t)=\int d\vec{r}\, r^L Y_{L0}(\Omega)\rho(\vec{r},t)$$

Fourier transformation into frequency domain gives

$$\tilde{D}(\omega)=\int dt\, e^{i\omega t} D(t)$$

TD-DFT formalism (3)

TD-DFT can be also formulated in terms of:
- **matrix RPA,**
- **separable RPA,**
- **strength function,**
- **….**

- **There are TD-DFT codes for spherical nuclei**

- **Only a few TD-DFT codes for deformed nuclei:**
  - **P.-G. Reinhard (Erlangen, Germany): full RPA with Skyrme forces, axial nuclei** → **- two weeks of calculation for one nucleus, -systematic calculations are impossible**
  - **Dubna: self-consistent separable RPA, with Skyrme forces, axial nuclei** → **- 20 minutes of calculation for one nucleus, -systematic calculations are welcome**
  - **S. Peru (Bruyères-le-Châtel, France) : RPA with Gogny forces, axial nuclei**

Separable self-consistent RPA (SRPA)

Time-dependent formulation:

$$E(J_\alpha(\vec{r},t)) = \langle \Psi | H | \Psi \rangle,$$

$$J_\alpha(\vec{r},t) \in \{\rho(\vec{r},t), \vec{j}(\vec{r},t), \ldots\} \qquad J_\alpha(\vec{r},t) = \langle \Psi | \hat{J}_\alpha | \Psi \rangle$$ ← T-even and T-odd densities

$$J_\alpha(\vec{r},t) = \bar{J}_\alpha(\vec{r}) + \delta J_\alpha(\vec{r},t)$$ ← Linear regime: small time-dependent perturbation

$$h(\vec{r},t) = h_0(\vec{r}) + \delta h_{res}(\vec{r},t)$$ ← Mean field hamiltonian: static g.s. + time-dependent response

$$= \sum_\alpha \left[\frac{\delta E}{\delta J_\alpha}\right]_{J=\bar{J}} \hat{J}_\alpha(\vec{r}) + \sum_{\alpha\alpha'} \left[\frac{\delta^2 E}{\delta J_\alpha \delta J_{\alpha'}}\right]_{J=\bar{J}} \delta J_\alpha(\vec{r},t) \hat{J}_\alpha(\vec{r})$$

$$\delta J_\alpha(t) = \langle \Psi(t) | J_\alpha | \Psi(t) \rangle - \langle 0 | J_\alpha | 0 \rangle$$ ← **The only unknowns**

Now we have to specify the perturbed many-body wave function Ψ

SRPA (2)

$$V_{res} \Rightarrow \sum_{k,k'=1}^{K} \{\kappa_{kk'} \hat{X}_k \hat{X}_{k'} + \eta_{kk'} \hat{Y}_k \hat{Y}_k\}$$

Macroscopic step:

Perturbed w.f. via scaling: $\Psi(t) = \prod_{k=1}^{K} \exp\{-q_k(t)\hat{P}_k\} \exp\{-p_k(t)\hat{Q}_k\} |0\rangle,$

both $\Psi(t), |0\rangle$ are Slater determinants

$$\hat{Q}_k = \hat{Q}_k^+, \quad \hat{T}\hat{Q}_k\hat{T}^{-1} = \hat{Q}_k$$
$$\hat{P}_k = i[\hat{H}, \hat{Q}_k]_{ph} = \hat{P}_k^+, \quad \hat{T}\hat{P}_k\hat{T}^{-1} = -\hat{P}_k$$

$$q_k(t) = \overline{q}_k \cos(\omega t)$$
$$p_k(t) = \overline{p}_k \sin(\omega t)$$

$$\hat{h}_{res}(t) = \sum_k \{-q_k(t)\hat{X}_k + p_k(t)\hat{Y}_k\} \overset{kk'}{=} 1/2 \sum_{kk'} \{\kappa_{kk'} \delta\hat{X}_k(t)\hat{X}_k + \eta_{kk'} \delta\hat{Y}_k(t)\hat{Y}_k\}$$

Microscopic step:

Perturbed w.f. via Thouless theorem: $\Psi_{Th}(t) = \{1 + \sum_{ph} c_{ph}(t)\hat{A}_{ph}^+)\} |0\rangle$

$$c_{ph}(t) = c_{ph}^+ e^{i\omega t} + c_{ph}^- e^{-i\omega t}$$

Joining step:

Both scaling and Thouless w.f. $\Psi(t)$ **must give equal variations:**

$$\delta\hat{X}_k(t)|_{sc} = \delta\hat{X}_k(t)|_{Th}, \quad \delta\hat{Y}_k(t)|_{sc} = \delta\hat{Y}_k(t)|_{Th}$$

SRPA (3)

V.O. Nesterenko, W. Kleinig,
J.Kvasil, P.-G. Reinhard, P. Vesely,
PRC, 66, 044307 (2002),
PRC, 74, 064306 (2006).

Final RPA equations:

$$\sum_k \{\overline{q}_k (d_{kk'}(XX) - \kappa^{-1}_{kk'}) + \overline{p}_k d_{kk'}(XY)\} = 0$$

$$\sum_k \{\overline{q}_k d_{kk'}(YX) + \overline{p}_k (d_{kk'}(YY) - \eta^{-1}_{kk'})\} = 0$$

T-even T-odd

$$H = h_0 + 1/2 \sum_{kk'} \{\kappa_{kk'} \hat{X}_k \hat{X}_{k'} + \eta_{kk'} \hat{Y}_k \hat{Y}_k\}$$

$$\det[\omega_j] = 0 \Longrightarrow \text{RPA spectrum}$$

where e.g. $$d_{kk'}(XY) = \sum_{ph} [\frac{\langle ph | \hat{X}_k | 0\rangle^* \langle ph | \hat{Y}_{k'} | 0\rangle}{(\varepsilon_{ph} - \omega)} + \frac{\langle ph | \hat{X}_k | 0\rangle \langle ph | \hat{Y}_{k'} | 0\rangle^*}{(\varepsilon_{ph} + \omega)}]$$

$$\hat{X}_k(\vec{r}) = i \sum_{\alpha\alpha'} [\frac{\delta^2 E}{\delta J_\alpha \delta J_{\alpha'}}] \langle 0 | [J_\alpha, \hat{P}_k] 0\rangle \hat{J}_{\alpha'}$$

$$\hat{Y}_k(\vec{r}) = i \sum_{\alpha\alpha'} [\frac{\delta^2 E}{\delta J_\alpha \delta J_{\alpha'}}] \langle 0 | [J_\alpha, \hat{Q}_k] 0\rangle \hat{J}_{\alpha'}$$

$$\kappa^{-1}_{kk'} = i \int d\vec{r} \langle 0 | [\hat{X}_k, \hat{P}_{k'}] | 0\rangle$$

$$\eta^{-1}_{kk'} = i \int d\vec{r} \langle 0 | [\hat{Y}_k, \hat{Q}_{k'}] | 0\rangle$$

$$C^+ = \sum_{ph} [c^-_{ph} a^+_p a_h - c^+_{ph} a^+_h a_p] \qquad \text{RPA phonon}$$

$$c^{\pm}_{ph} = -\frac{1}{2} \frac{\sum_k \{\overline{q}_k \langle ph | \hat{X}_k | 0\rangle \mp i \overline{p}_k \langle ph | \hat{Y}_k | 0\rangle\}}{\varepsilon_{ph} \pm \omega}$$

- Rank of RPA matrix is 4K.
For giant resonances
usually K=2 is enough.
Very low rank!

SRPA (5)

Lorentz weight

$$\xi(\omega-\omega_\nu)=\frac{1}{2\pi}\frac{\Delta}{(\omega-\omega_\nu)^2+(\Delta/2)^2}$$

L=0,1,3

Strength function:

$$S_L(D_{X\lambda\mu})=\sum_\nu \omega_\nu^L \,<\nu|\hat{D}_{X\lambda\mu}|0>^2\ \xi(\omega-\omega_\nu)=$$

$$=\underbrace{\frac{1}{\pi}\Im\left[\frac{z^L\sum_{\beta\beta'}F_{\beta\beta'}(z)A_\beta(z)A_{\beta'}(z)}{F(z)}\right]_{z=\omega+i\Delta/2}}_{\text{Contribution of residual inter.}}+\underbrace{\sum_{ph}\varepsilon_{ph}^L<ph|\hat{D}_{X\lambda\mu}|0>^2\ \xi(\omega-\omega_\nu)}_{\text{Unperturbed 2qp strength}}$$

Alternative separable RPA methods with Skyrme/Migdal forces:

- N.Van Giai, Ch.Stoyanov, V.V.Voronov, PRC, 57, 1204 (1998)
- A.P.Severyuchin, Ch.Stoyanov, V.V.Voronov, N.Van Giai, PRC, 66,034304 (2002)

(-)) Larger rank of RPA matrix, K=400
(-) No T-odd densities
(+) No problem with the choise of initial operators

How to choose the proper Skyrme force?

One should take into account the bias of the force

Force		
SkT6 (1984), SkSC, MSk (2000)	- nuclear masses (m*/m = 1.00 - 1.05)	→ s-p spectra
SkM* (1982)	- isoscal. E2 giant resonance, fission barriers (m*/m = 0.79)	→ Isoscalar E2 GR, low-energy vibr. states
SLy6 (1997)	- isovector properties of nuclear matter (m*/m = 0.69)	→ isovector E1 GR

It is seen that isoscalar effective mass m*/m is a basic feature to classify Skyrme forces

Skyrme forces: isoscalar effective mass m*/m

Origin of m*/m in Skyrme forces:

$$\tau_q\{\frac{\hbar^2}{2m}+\frac{1}{8}\rho[t_1(2+x_1)+t_2(2+x_2)+\frac{1}{8}\rho_q[t_2(1+2x_2)-t_1(1+2x_1)]\}=\frac{\hbar^2}{2m_q^*}\tau_q$$

For symmetric nuclear matter

$$\rho_p=\rho_n=\rho/2$$

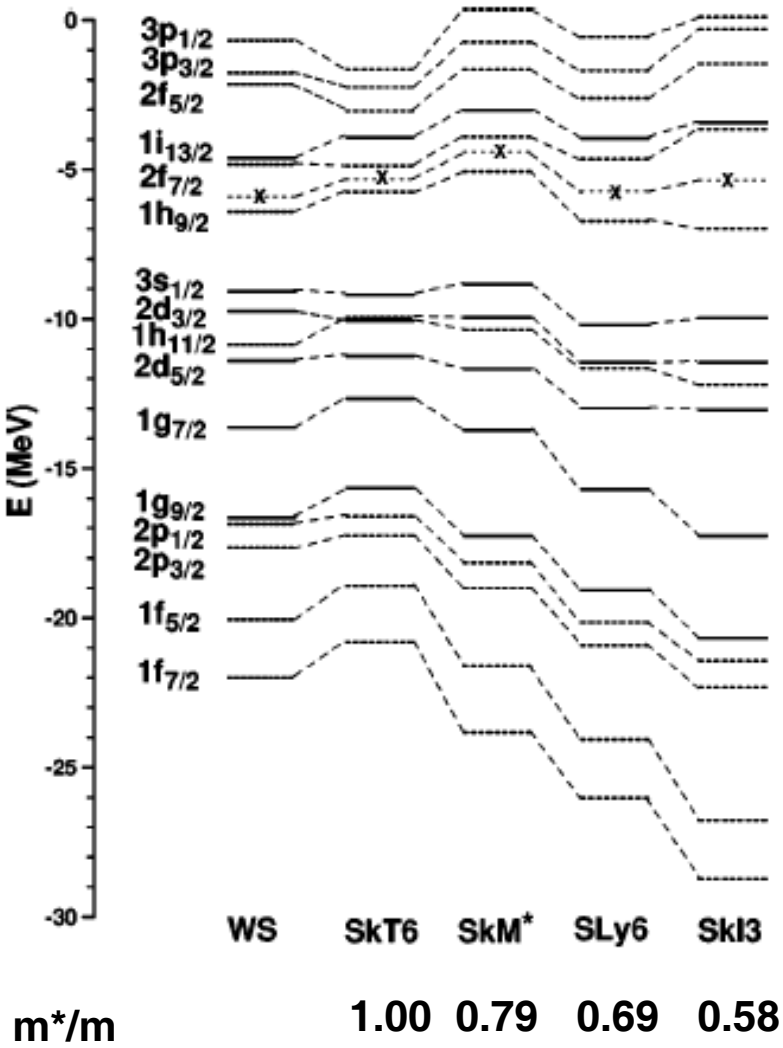
and so

$$(m^*/m)^{-1}=1+\frac{1}{8}\frac{m}{\hbar^2}\rho[3t_1+t_2(5+4x_2)]$$

Isoscalar effective mass depends on coordinates in finite nuclei and constant in nuclear matter.

Skyrme forces: isoscalar effective mass m*/m

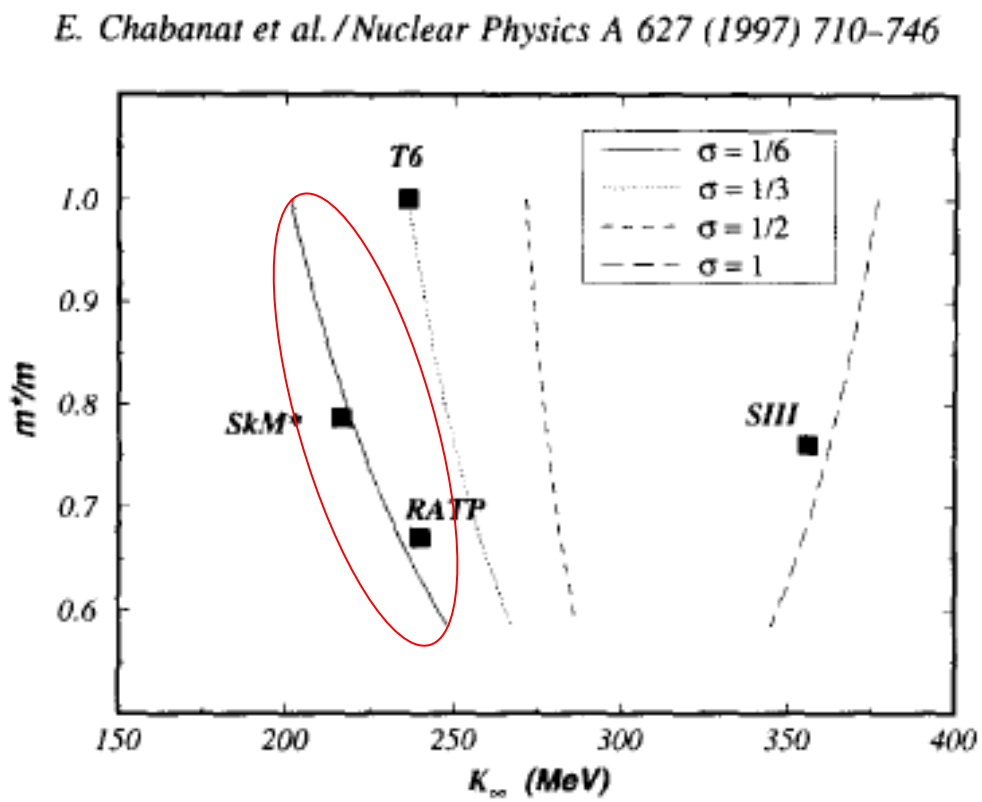
V.O. Nesterenko et al,
PRC, 70 (2004) 057304



Isoscalar effective mass dramatically changes s-p spectrum while keeping the same s-p w.f..

The lower m*/m, the more dilute the s-p spectrum

- **Isoscalar effective mass is related with incompressibility K**



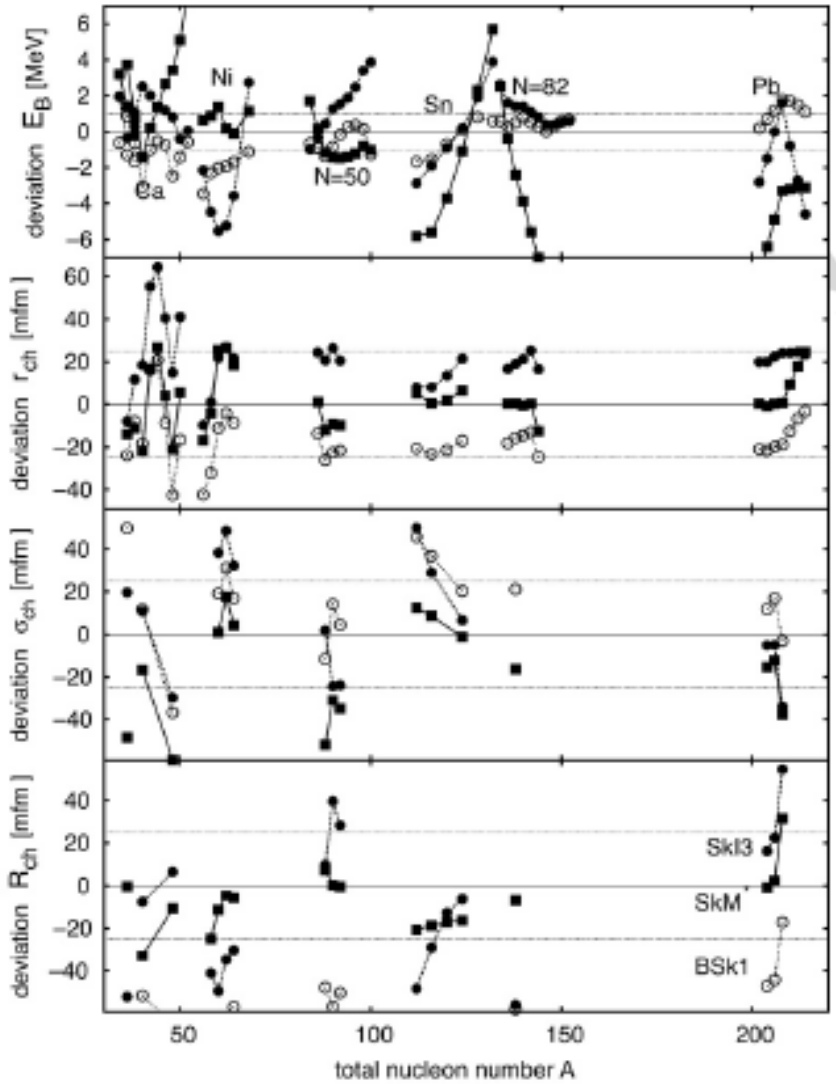
- **Relation of isoscalar** m_0^*/m **and isovector** m_1^*/m **effective masses?**

W. Satula et al, PRC, 74 (2006) 011301.

Application of SF to finite nuclei: ground state

Skyrme forces
BSk1, SkM*, SKI3

Deviation between experiment and theory: $\delta = O_{\exp} - O_{theor}$



$E_B[MeV]$ **- binding energy per nucleon**

$\delta \sim \pm 1\text{MeV}, \quad 0.006\%$

$r_{ch}[mfm]$ **- r.m.s. radius**

$\delta \sim \pm 0.025\,\text{fm}, \quad 0.003\%$

$\sigma_{ch}[mfm]$ **- surface thickness**

$R_{ch}[mfm]$ **- difraction radius**

J.R. Stone, P.-G. Reinhard
Prog. Part. Nucl. Phys., 58 (2007) 587-657.

Isovector E1 giant resonance

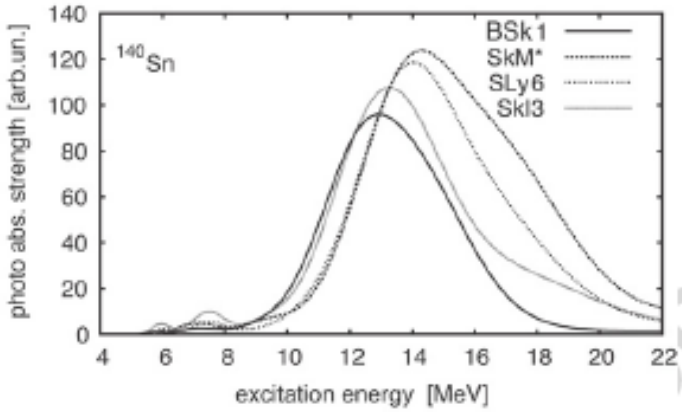


Fig. 10. The photo-absorption strength for ^{140}Sn computed with RPA using four different Skyrme parameterizations as indicated. The self-consistent RPA techniques from [157,158] have been used. The spectra are folded with a Gaussian width of $\Gamma = (E_n - \varepsilon_{F,neutr}) * 0.2$ MeV to simulate escape and collisional broadening.

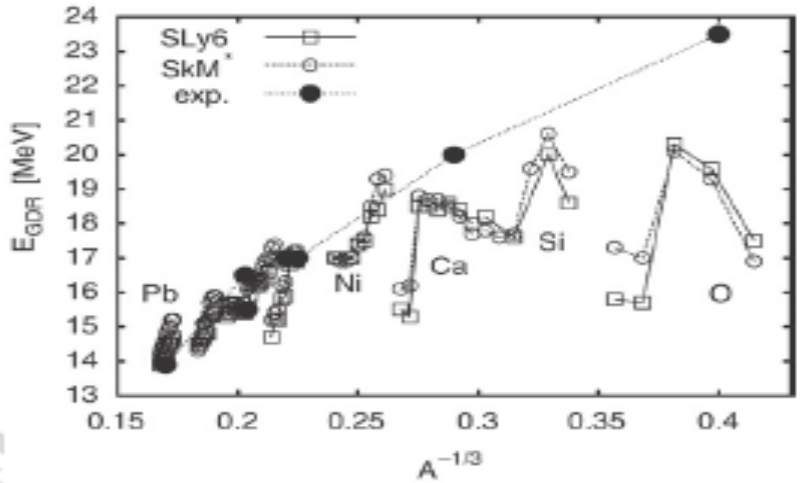
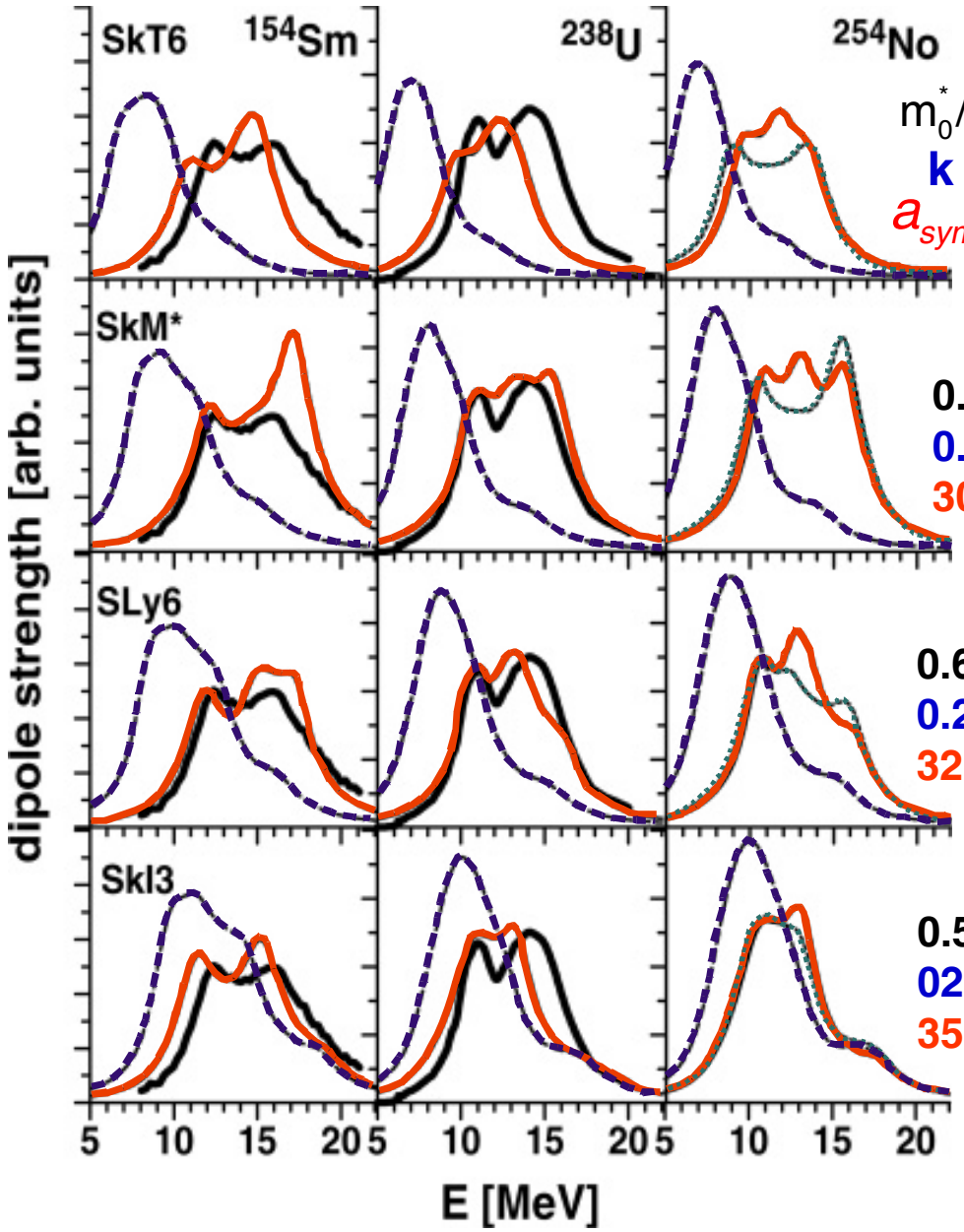


Fig. 12. The average peak position of the giant dipole resonance in a broad range of spherical nuclei drawn versus $A^{-1/3}$ (which is proportional to the inverse radius). Results are shown for two different Skyrme forces as indicated and compared with experimental data where available.

E1 (T=1)resonance in photoabsorption [dependence on Skyrme force]

V.O. Nesterenko, et al, PRC,74, 064306 (2006).



m_0^*/m= 1.00
k = 0
a_{sym} = 30

0.79
0.53
30

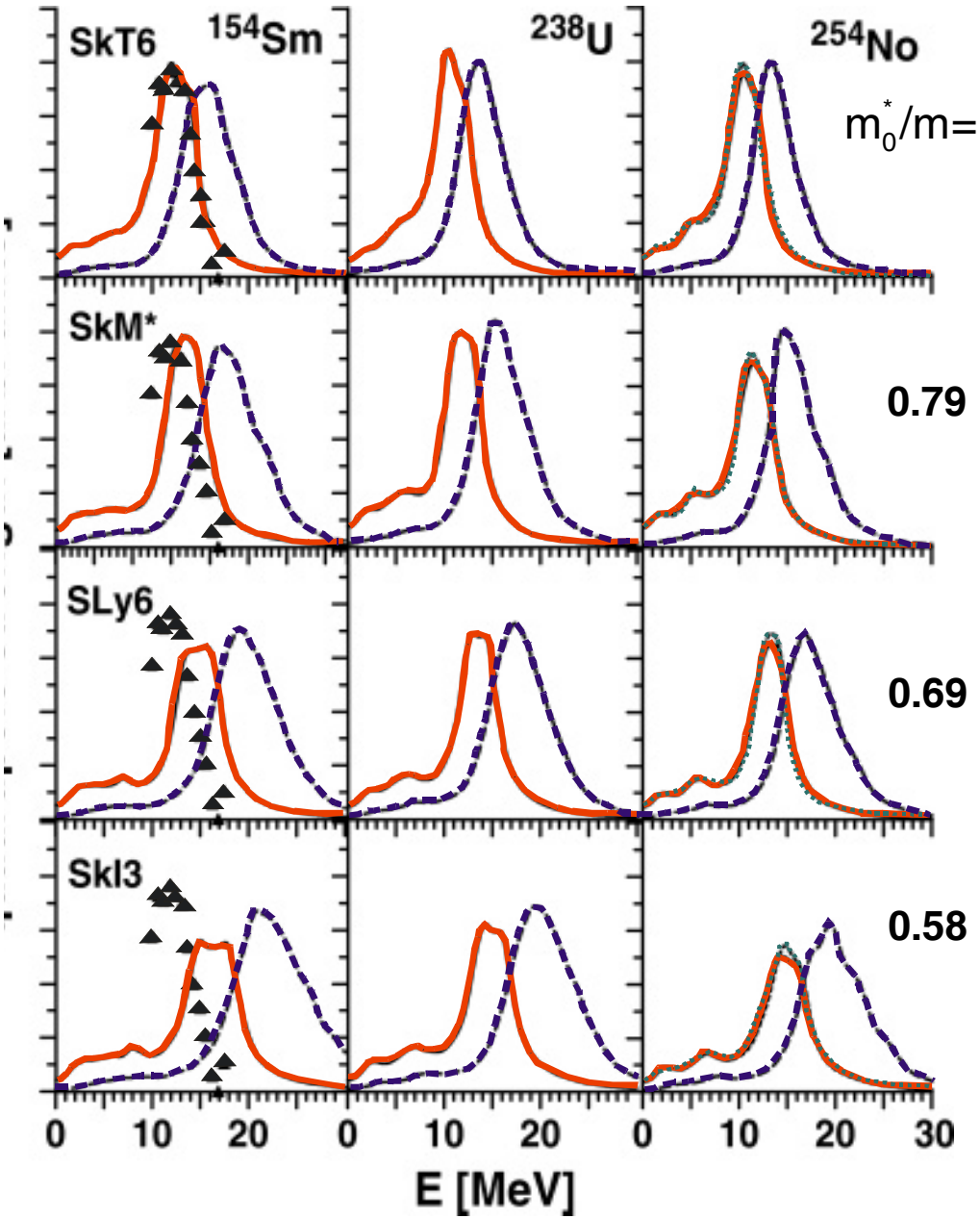
0.69
0.25
32

0.58
025
35

—— exper.
—— unperturbed 2qp (without res. Inter.)
—— SRPA

- Good agreement with experiment in general. Best for SLy6.
- Dependence of 2qp strength and collective shift on m_0^*/m
- SkM*: artificial right shoulder, 3-peak structure. Reason: high k= 0.53 and hence too large collective shift.
- Right flank of E1(T=1) is very sensitive to forces. This feature can be used for their upgrade.
- E1(T=1) energy decreases with a_{sym} in contrast with macrosc. theory. Density dependent a_{sym} !
- No peculiarities for superheavy 254No

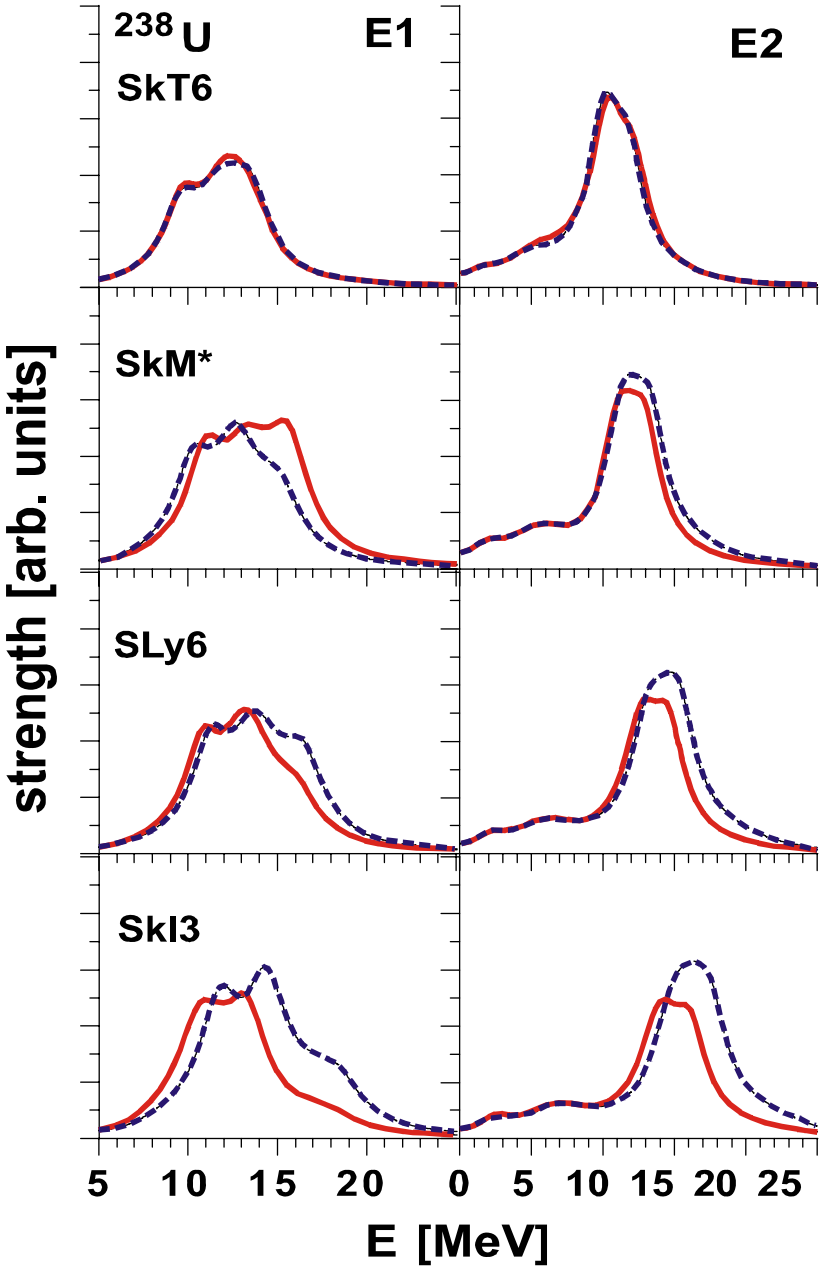
E2(T=0) resonance (exp.: (α,α) , Youngblood,2004)
Dependence on Skyrme force



▲▲▲ exper.
——— unperturbed 2qp (without res. Inter.)
——— SRPA

- Dependence of 2qp strength and collective shift on m^*_0/m
- Best agreement with experiment for SkT6 and SkM*. E2(T=0) likes high m^*_0/m
- Simultaneous description of E1(T=1) and E2(T=0) GR need Skyrme forces with high m^*_0/m (SkM*) and modest isovector characteristics (SLy6). Development of such forces is now in progress.

E1(T=1)and E2(T=0) resonances: contribution of time-odd current to residual interaction



···· without current
— with current

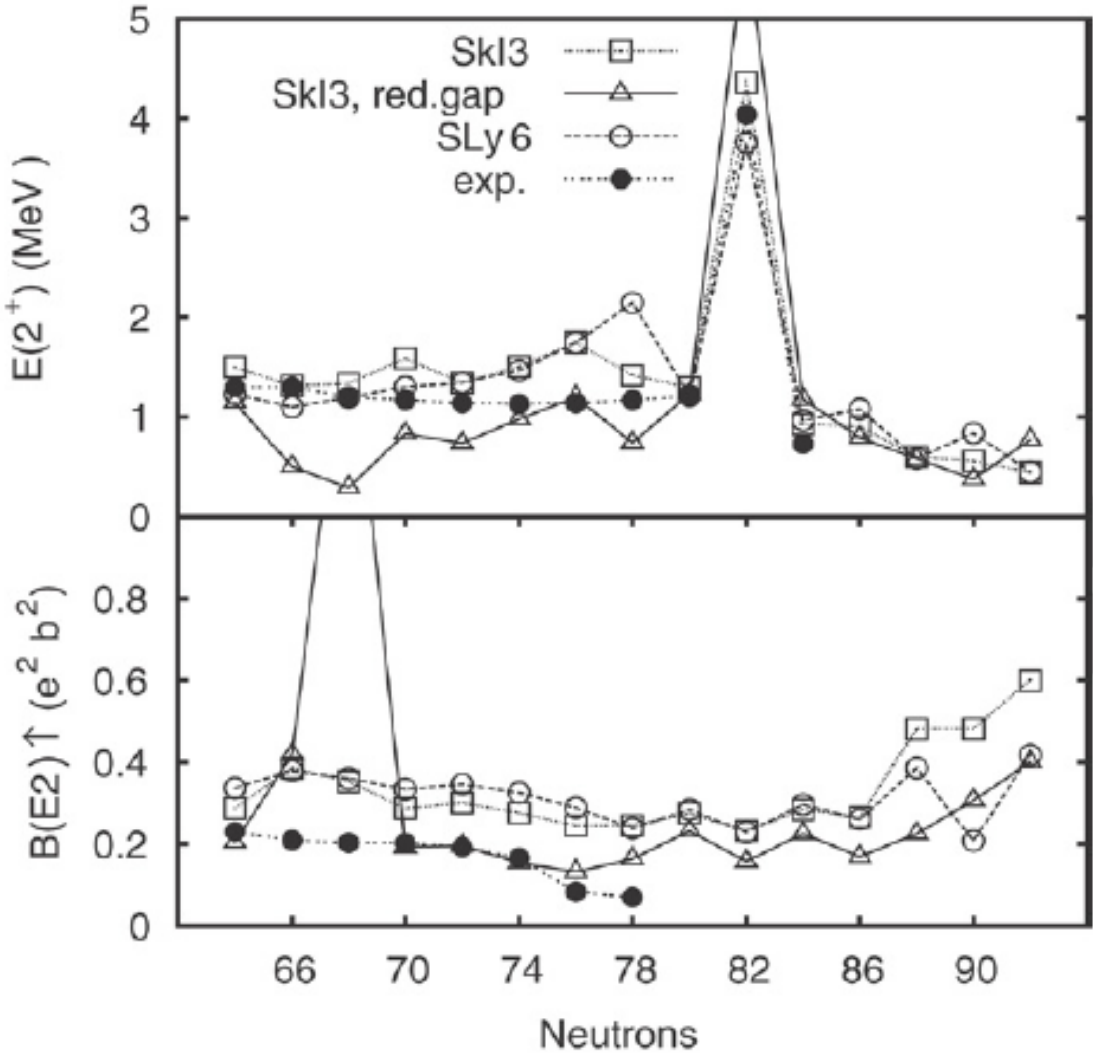
$$b_1(\rho\tau - \vec{j}^2) - b'_1 \sum_s (\rho_s\tau_s - \vec{j}_s^2)$$

- Again right flank is mainly affected.
- Strong effect, especially for low m_0^*/m and high m_1^*/m. Regular trend for E2 and irregular for E1.
- No impact at all for SkT6 with m*/m=1
- Correlations between time-odd impact and effective masses. Such correlations are natural since both factors originate from one term of Skyrme functional

$$\sim b_1, b'_1$$

- GR are good to test time-odd effects.

Application of SF to finite nuclei:
low-energy vibrational states



low-energy 2^+ states in the chain of Sn isotopes

Δ - 75% reduced pairing strength

No calculations for low-energy vibrational states in deformed nuclei (rare-earth and actinide regions)

Equation of state (EOS)

Nuclear matter obeys thermodynamical relation between pressure P and Helmholz free energy F = E-TS:

$$P = \frac{\partial F}{\partial V}\Big|_{T,s} \longrightarrow \underbrace{P = n^2 \frac{\partial \varepsilon(n,I)}{\partial n}\Big|_I}_{\text{EOS}} \quad \text{for T=0}$$

EOS ← relates preasure and energy/density, very important for astrophysical models

n – density

$I = \frac{N-Z}{A} = \frac{n_n - n_p}{n}$ **- asymmetry parameter**

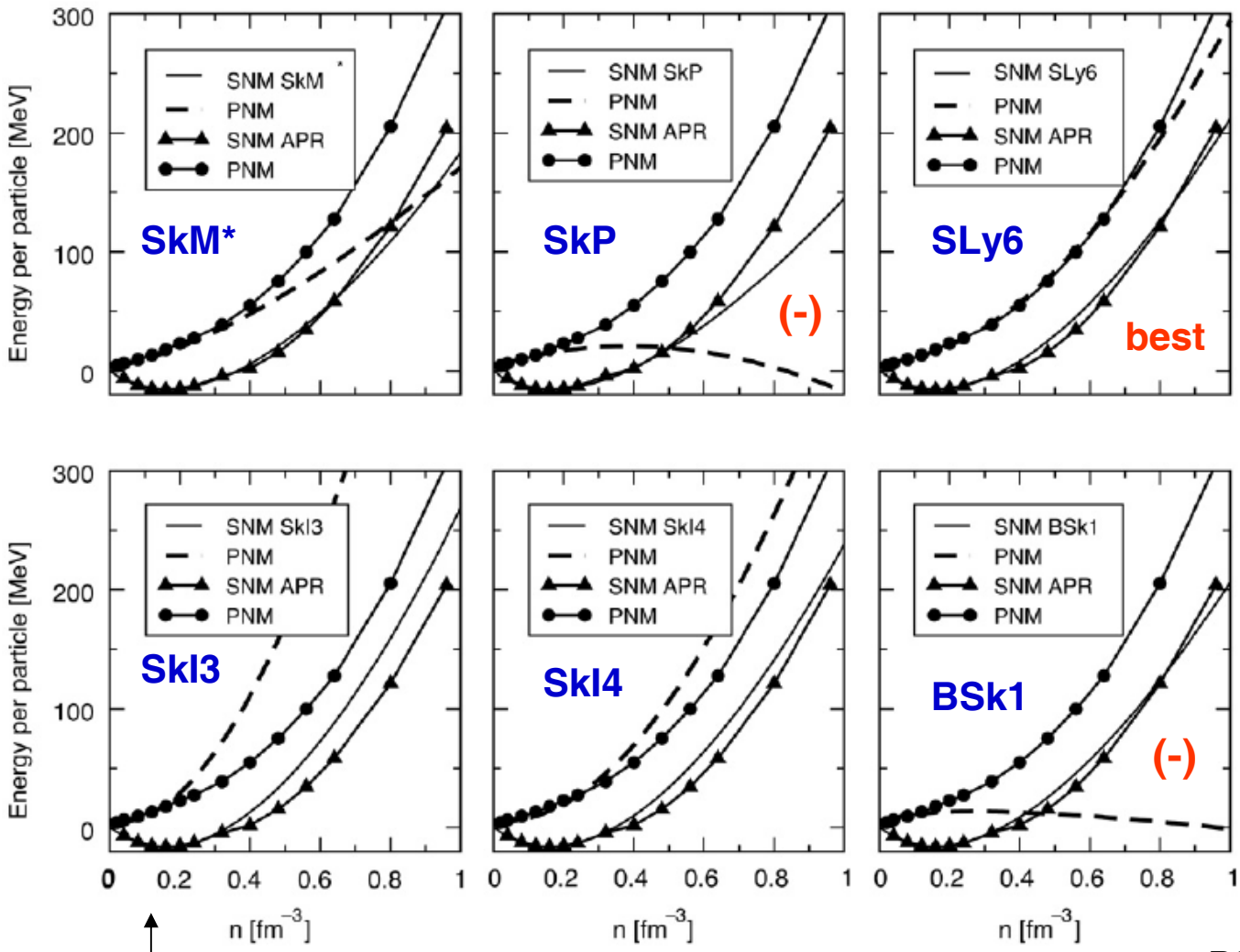
I = 0 – symmetric nuclear matter (SNM)
I = 1 – pure neutron matter (PNM)

$\varepsilon(n,I)$ **- binding energy per particle (important for EOS!)**

"Experimental" benchmark: ab initio calculations with realistic potential
A18 +δv+UIX*(APR)
based on Argonne A18 two-body inter.
+ three-body inter. UIX*

J.R. Stone, P.-G. Reinhard, 2007

Skyrme forces to NM: binding energy



$n_0 = 0.16 \pm 0.005$ fm^{-3}

SLy6 is maybe the best force for drip-line nuclei, neutron stars

-6 Skyrme forces:
SkM*, SkP, SLy6
SkI3, SkI4, BSk1

vs

APR results for SNM, PNM

SNM:
good agreement for all forces for low density, not for high density

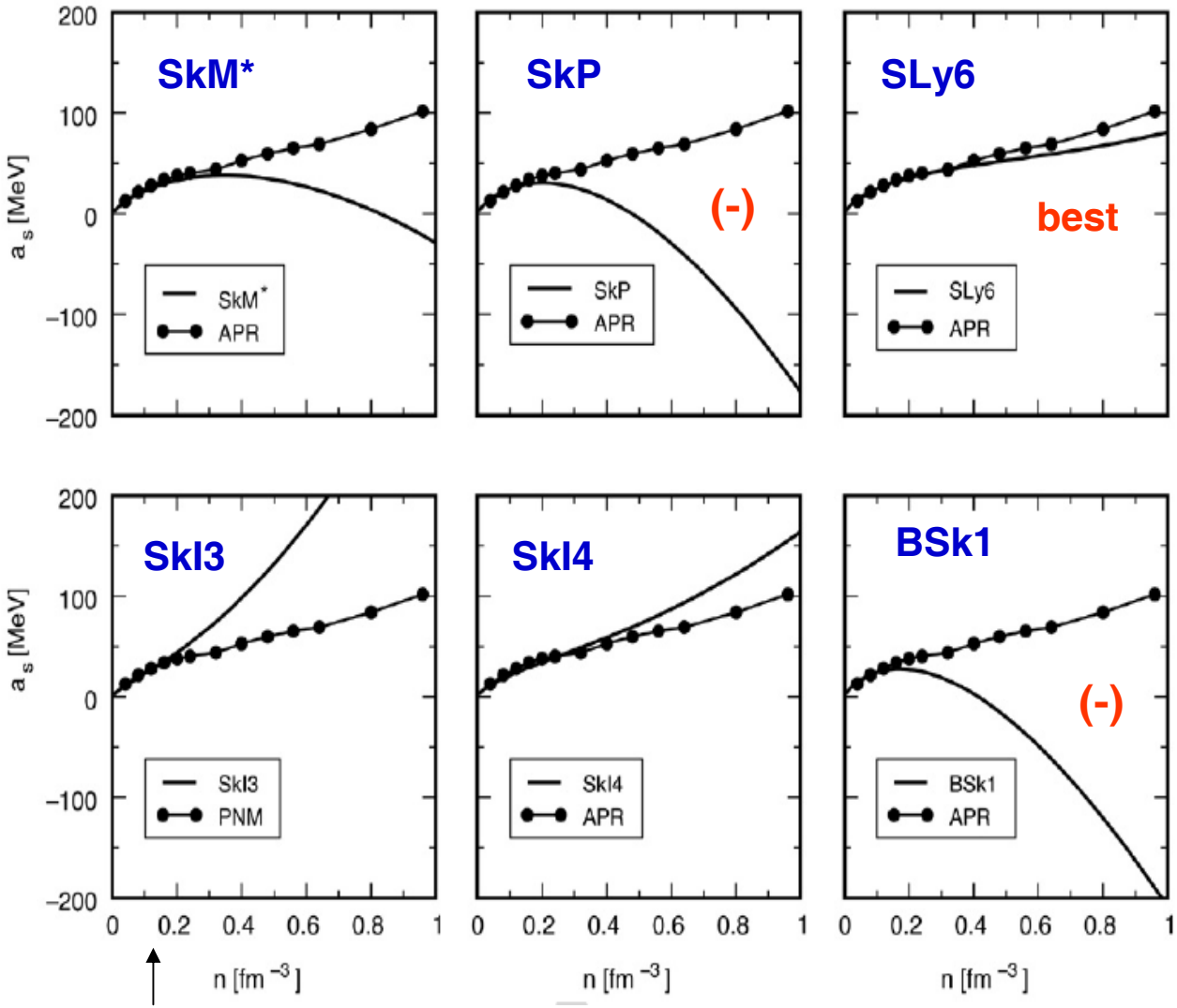
PNM:
agreement only for SLy6

BSk1 (2002) is fitted Exclusively to binding energies (= nuclear masses)

Skyrme forces for NM: asymmetry

J.R. Stone, P.-G. Reinhard, 2007

$$E_{sym} = a_{sym}\frac{(N-Z)^2}{A^2} = a_{sym}\, I^2$$



$n_0 = 0.16 \pm 0.005$ fm^{-3}

asymmetry coeff:

$$a_{sym} = \frac{1}{2}\frac{d^2\varepsilon}{dI^2} = \frac{n^2}{2}\frac{d^2\varepsilon}{dn_{iv}^{\,2}}$$

Again SLy6 is best

The forces SkP, BSk1 give unphysical results:
- the g.s.for PNM,
- pressure <0, collapse

Forces SkP, BSk1 cannot be used for astrophysical (maybe drip-line) problems

Observables of cold (T=0) neutron stars

J.R. Stone, P.-G. Reinhard, 2007

Table 2

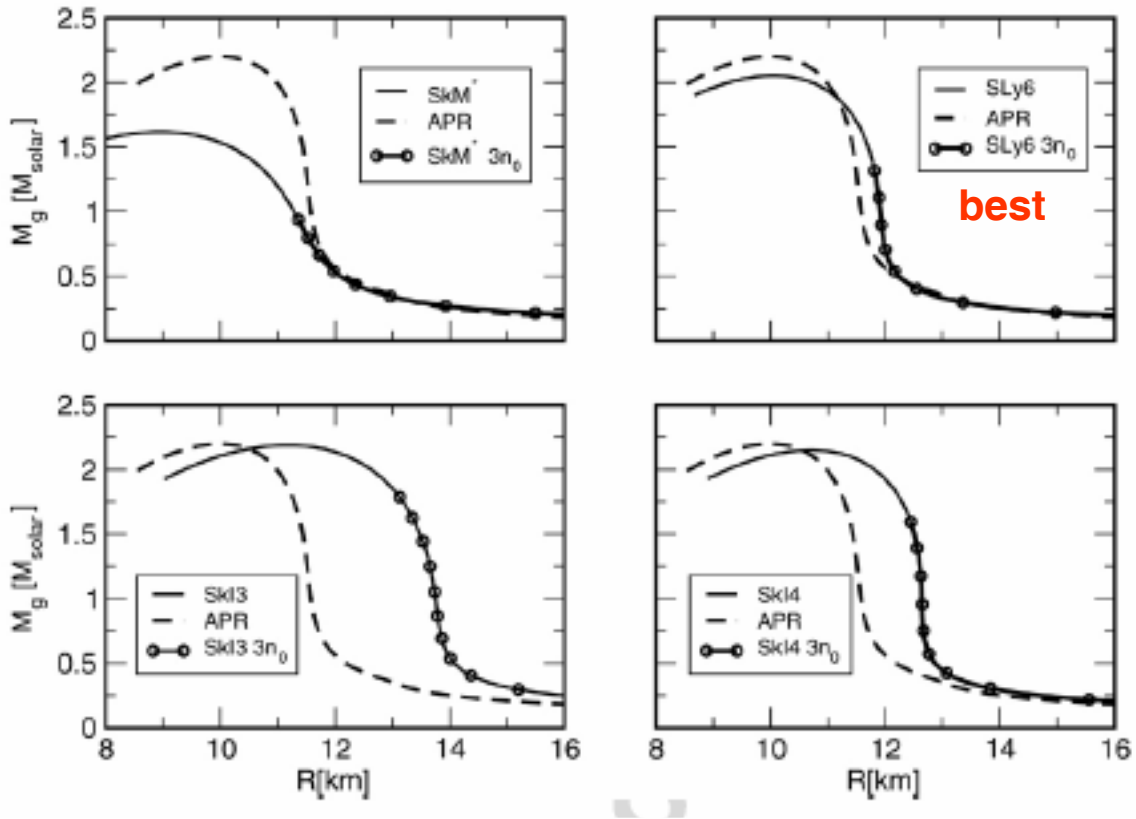
Observables of nuclear matter and cold ($T = 0$) non-rotating neutron stars: Calculated maximum mass with corresponding radius and central density, and the radius and binding energy of a 1.4 $M_\odot$ star for Skyrme functionals SkM*, SkP, SLy6, SkI3, SkI4 and BSk1

EoS	$a_s(n_0)$ (MeV)	$a_s(3n_0)$ (MeV)	$\frac{\partial a_s}{\partial n}(n_0)$	M_{max} ($M_\odot$)	R_{max} (km)	n_{max}^{centr} (fm^{-3})	ρ_{max}^{centr} (g/cm^3)	$R_{1.4\,M_\odot}$ (km)	E_{bin} (10^{53} ergs)
SkM*	30.01	34.02	+95	1.62	8.94	1.66	3.80	10.54	3.09
SkP	29.71	−0.43	+43	0.60	814				
SLy6	32.09	51.84	+99	2.05	10.05	1.19	2.82	11.76	2.58
SkI3	34.27	125.00	+212	2.19	11.19	0.98	2.33	13.56	2.18
SkI4	29.50	98.85	+125	2.15	10.71	1.05	2.49	12.56	2.43
BSk1	27.86	−15.06	+12	0.61	1089				
FP	31	40		1.95	9.0	1.3			
APR	33.94	59.67		2.20	10.01	1.14	2.73	11.47	2.75
BJ				1.85	9.90	1.31	3.06	11.86	2.51
Hybrid				1.45	10.45	1.36	2.76	11.38	2.49

The symmetry energy at saturation density n_0, $3n_0$ and the derivative of the symmetry energy at the saturation density $\partial a_s/\partial n(n_0)$ are also given. Results for four other EoS based on different models of the nucleon–nucleon interaction, are added for comparison. See text for more explanation.

Cold neutron star: maximal gravitational mass vs maximal radius

Tolman-Oppenheimer-Volkov equation.



Most of Skyrme forces well describe:

- **g.s. properties of finite nuclei**
- **symmetric nuclear matter at saturation density**

but only a few Skyrme forces can describe

- **SNM at high densities**
- **pure neutron matter**
- **basic characteristics of cold neutron stars**

J.R. Stone, P.-G. Reinhard, 2007

Basic NM values:

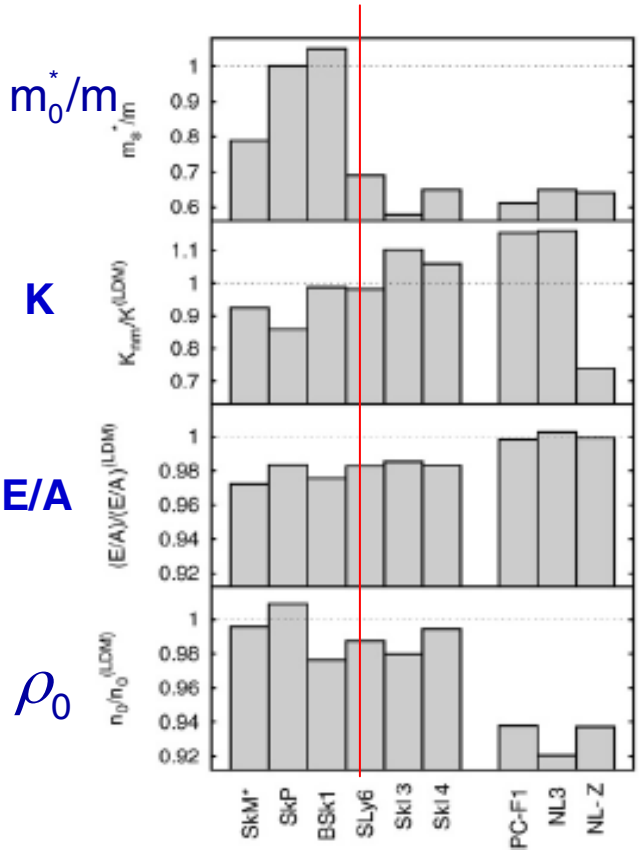
LD model vs Skyrme (SkM*, SkP, BSk1, SLy6, SkI3, SkI4) and RMF (PCF1,NL3,NL-Z)

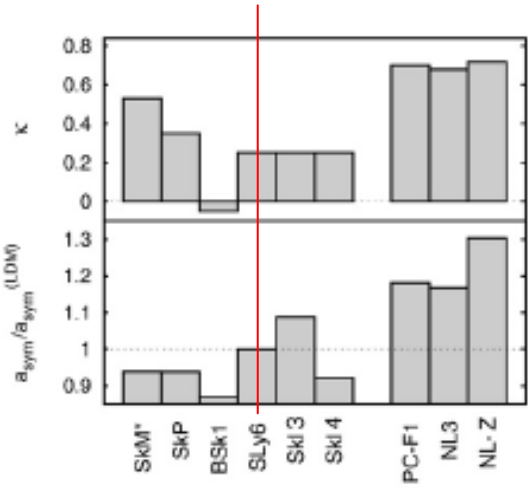
m_0^*/m

K

E/A

ρ_0





a_{sym}

$k \rightarrow m_1^*/m = \frac{1}{1+k}$

- SMF agrees bettter with LD and hence has better credibility than RMF

- SMF/RMF strictly deviate for:
  - effective masses,
  - saturation densities,
  - asymmetries

- RMF is not flexible in isovector channel, needs essential modifications

Summary

DFT, TD-DFT are now basic theoretical tools in physics of nuclear and electronic systems.

Optimal compromise between simplicity and realistic results.
Good perspectives for further progress.

DFT with Skyrme forces is one of the most promising models:
- **pretend to describe finite nuclei (+ exotic), nuclear matter, neutron stars, …**
- **still too many parametrizations,**
  though there are already a few quite reliable forces (SLy6, …)
- **useful for astrophysics**
- **rapid progress**