密度汎関数理論による計算核データ

Takashi NAKATSUKASA

Theoretical Nuclear Physics Laboratory

RIKEN Nishina Center

•DFT (Hohenberg-Kohn) → Static properties, EOS

•TDDFT (Runge-Gross) → Response, reaction

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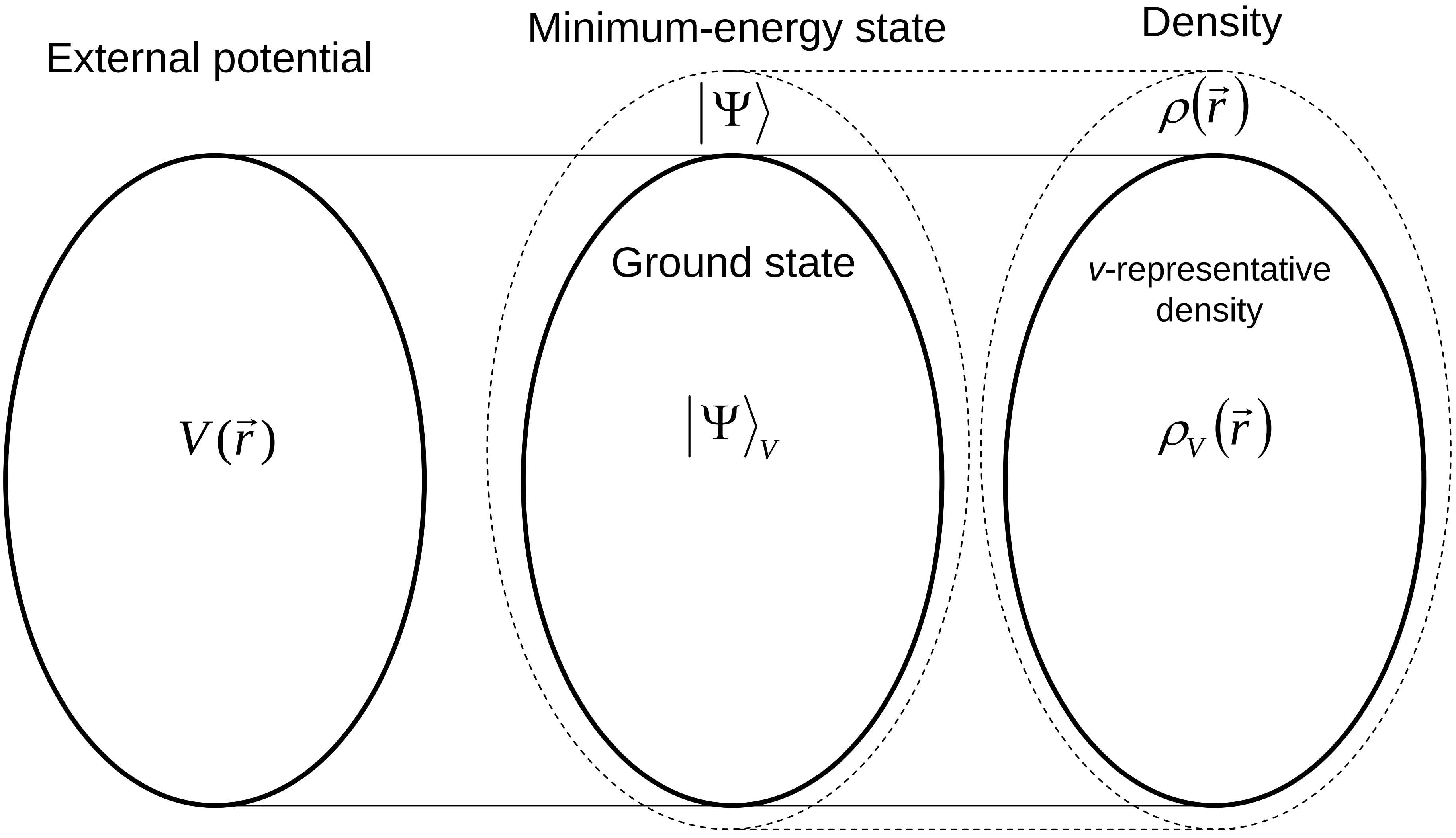
自己紹介

- 中務　孝（なかつかさ　たかし）
- 所属
  - 理研・仁科センター・中務原子核理論研究室
- 研究分野
  - 高スピン・超変形状態における核構造
  - 時間依存密度汎関数理論を用いた原子核・原子・分子・クラスター等の量子ダイナミクス計算
  - 大振幅集団運動理論
  - 実時間計算による3体量子反応計算
- HP
  - http://ribf.riken.jp/~nakatsuk/

One-to-one Correspondence



The following variation leads to all the ground-state properties.

$$\delta\left\{ F[\rho]+\int \rho(\vec{r})v(\vec{r})d\vec{r}-\mu\left(\int \rho(\vec{r})d\vec{r}-N\right)\right\}=0$$

In principle, any physical quantity of the ground state should be a functional of density.

Variation with respect to many-body wave functions $\Psi(\vec{r}_1,\cdots,\vec{r}_N)$

$\downarrow$

Variation with respect to one-body density $\rho(\vec{r})$

$\downarrow$

Physical quantity $A[\rho(\vec{r})]=\left\langle \Psi[\rho]\middle|\hat{A}\middle|\Psi[\rho]\right\rangle$

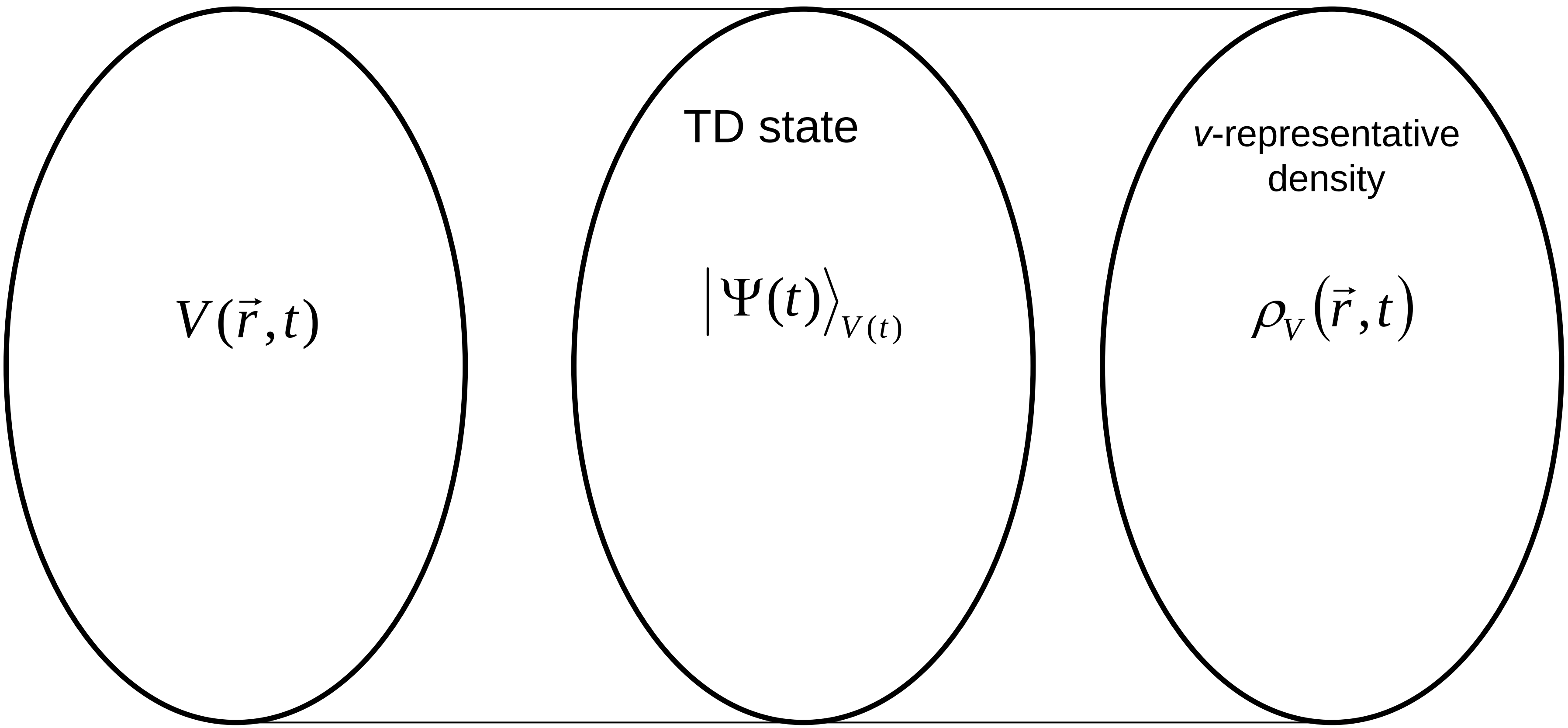
One-to-one Correspondence

External potential

Time-dependent state starting from the initial state

$$\left|\Psi(t_0)\right\rangle$$

Time-dependent density



The universal density functional exists, and the variational principle determines the time evolution.

From the first theorem, we have $\rho(\boldsymbol{r},t) \leftrightarrow \Psi(\mathrm{t})$. Thus, the variation of the following function determines $\rho(\boldsymbol{r},t)$.

$$S[\rho] = \int_{t_0}^{t_1} dt \left\langle \Psi[\rho](t) \middle| i\frac{\partial}{\partial t} - H(t) \middle| \Psi[\rho](t) \right\rangle$$

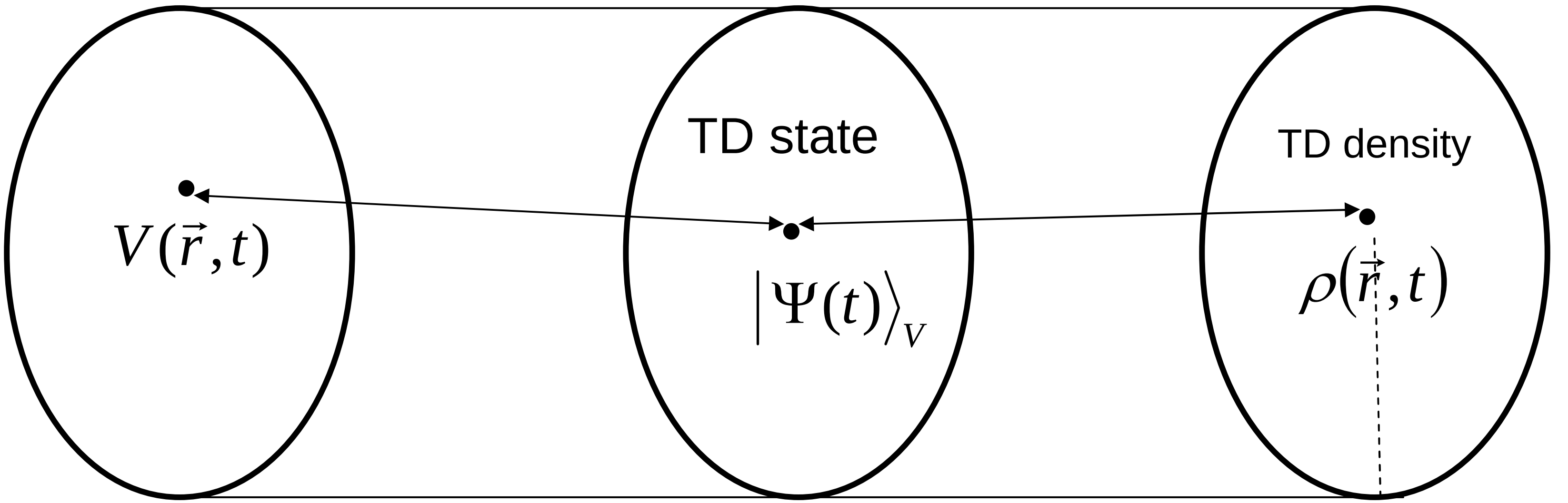
$$S[\rho] = \tilde{S}[\rho] - \int_{t_0}^{t_1} dt \int d\mathbf{r}\, \rho(\mathbf{r},t) v(\mathbf{r},t)$$

The universal functional $\tilde{S}[\rho]$ is determined.

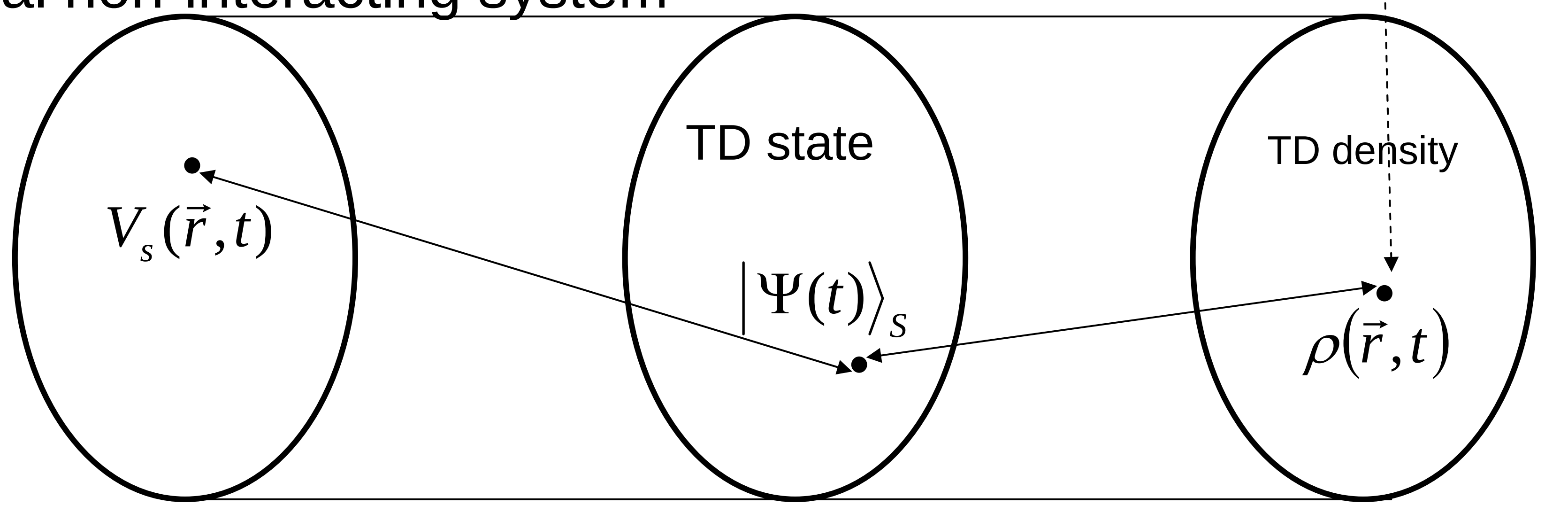
v-representative density is assumed.

TD Kohn-Sham Scheme

Real interacting system



Virtual non-interacting system



Time Domain	Energy Domain
Basic equations	**Basic equations**
• Time-dep. Schroedinger eq.	• Time-indep. Schroedinger eq.
• Time-dep. Kohn-Sham eq.	• Static Kohn-Sham eq.
• $d\boldsymbol{x}/dt = A\boldsymbol{x}$	• $A\boldsymbol{x}=a\boldsymbol{x}$ (Eigenvalue problem)
	• $A\boldsymbol{x}=b$ (Linear equation)
Energy resolution	**Energy resolution**
$\Delta E \sim \hbar / T$	$\Delta E \sim 0$
All energies	A single energy point
Boundary Condition	**Boundary condition**
• Approximate boundary condition	• Exact scattering boundary condition is possible
• Easy for complex systems	• Difficult for complex systems

How to incorporate scattering boundary conditions ?

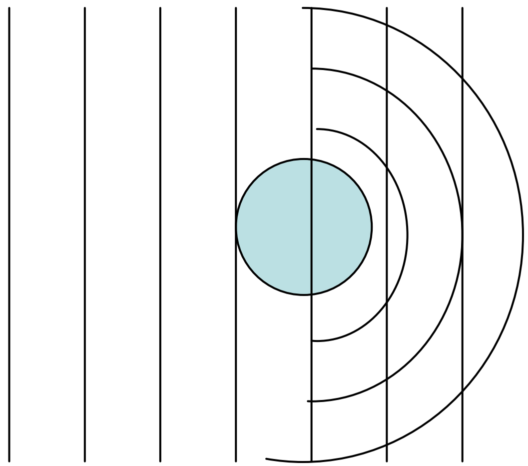
- It is automatic in real time !
- Absorbing boundary condition

Potential scattering problem

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\phi^{(+)}(\vec{r}) = E\,\phi^{(+)}(\vec{r})$$

$$\phi^{(+)}(\vec{r}) \underset{r\to\infty}{\longrightarrow} e^{ikz} + f(\Omega)\frac{e^{ikr}}{r}$$

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2$$



For spherically symmetric potential

$$\phi^{(+)}(\vec{r}) = \sum_l \frac{u_l(r)}{r} P_l(\cos\theta)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right]u_l(r) = Eu_l(r)$$

$$u_l(0) = 0, \qquad u_l(r) \underset{r\to\infty}{\longrightarrow} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

Phase shift δ_l

Time-dependent picture

$$\phi^{(+)}(\vec{r}) = e^{ikz} + \frac{1}{E+i\varepsilon-T}V(r)\phi^{(+)}(\vec{r})$$
$$= e^{ikz} + \frac{1}{E+i\varepsilon-H}V(r)e^{ikz}$$

Scattering wave

$$\chi(\vec{r}) = \frac{1}{E+i\varepsilon-H}V(r)e^{ikz} \quad \xrightarrow[r\to\infty]{} f(\Omega)\frac{e^{ikr}}{r}$$

$$\chi(\vec{r}) = \boxed{\frac{1}{E+i\varepsilon-H}}V(r)e^{ikz} = \boxed{\frac{1}{i\hbar}\int_0^\infty dt\, e^{i(E+i\varepsilon)t/\hbar}e^{-iHt/\hbar}}V(r)e^{ikz}$$

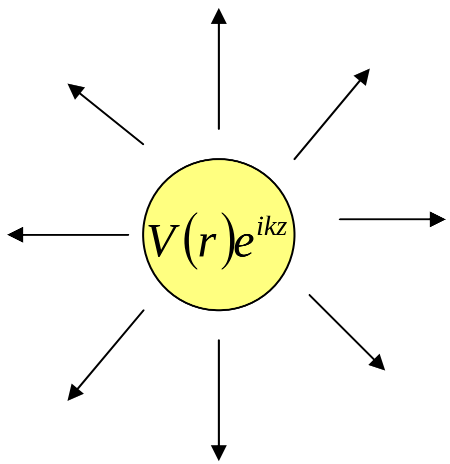
Time-dependent scattering wave

$$\psi(\vec{r},t=0) = V(r)e^{ikz}$$

(Initial wave packet)

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$

(Propagation)



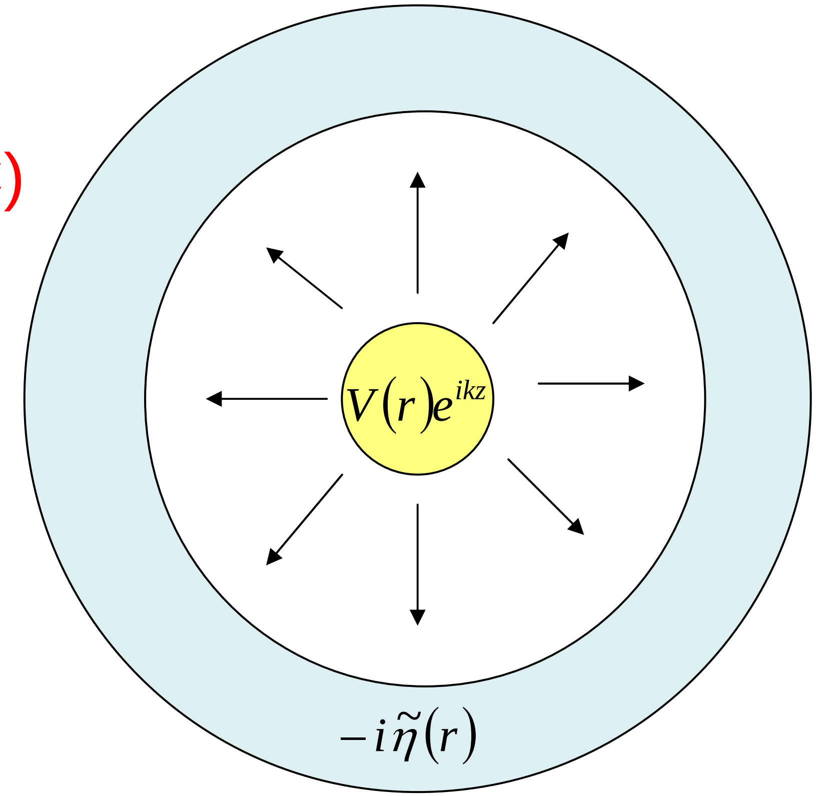
Projection on *E* : $\chi(\vec{r}) = \frac{1}{i\hbar}\int_0^\infty dt\, e^{iEt/\hbar}\psi(\vec{r},t)$

Boundary Condition

Absorbing boundary condition (ABC)

Absorb all outgoing waves outside the interacting region

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \left(H - i\tilde{\eta}(r)\right)\psi(\vec{r},t)$$



How is this justified?

$$f(\Omega) = -\frac{m}{2\pi\hbar^2}\int d\vec{r}\, e^{-i\vec{k}_\Omega \vec{r}} V(r)\phi^{(+)}(\vec{r})$$

$$\langle \mathbf{k}'|S|\mathbf{k}\rangle = \delta(\mathbf{k}'-\mathbf{k}) + 2\pi i\delta(E'-E)\langle \mathbf{k}'|V|\phi^{(+)}\rangle$$

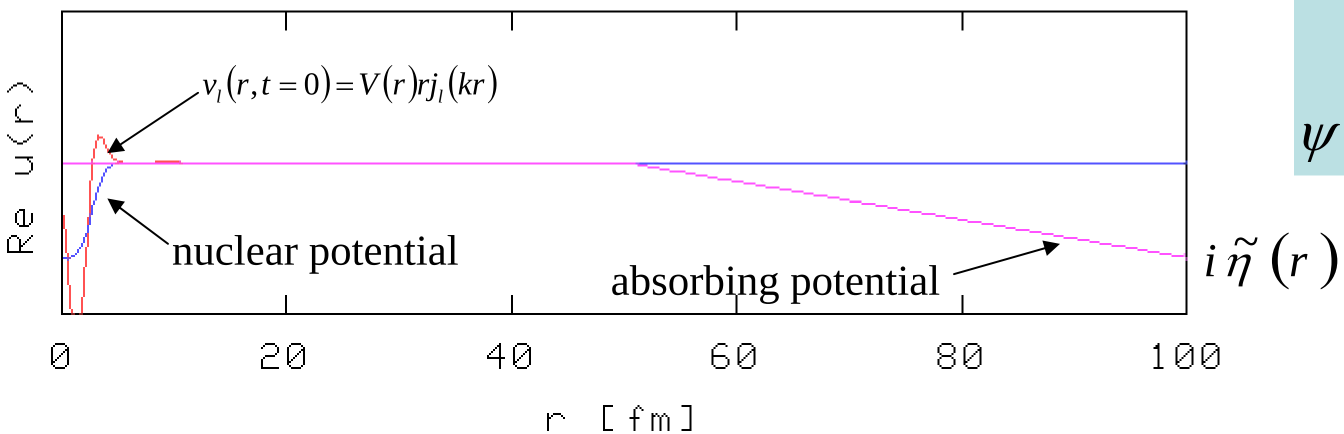
Finite time period up to *T*

Time evolution can stop when all the outgoing waves are absorbed.

$$\chi(\vec{r}) = \frac{1}{i\hbar}\int_0^T e^{iEt/\hbar}\psi(\vec{r},t)$$

s-wave

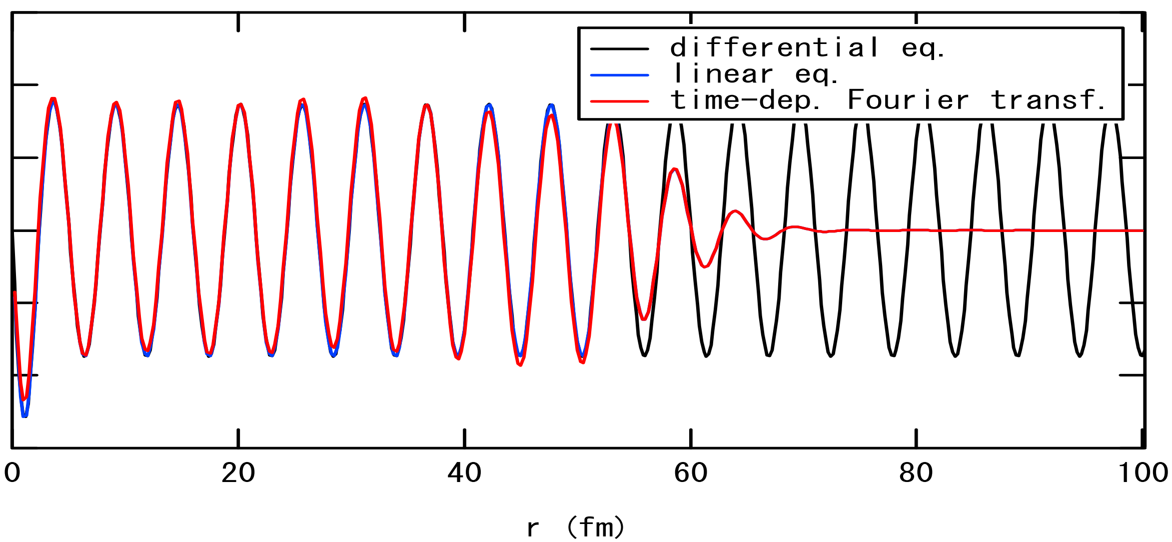
$$\mathrm{Re}\left[\psi(\vec{r},t)_{\ell=0}\right]$$



$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=H\psi(\vec{r},t)$$

$$\psi(\vec{r},t=0)=V(r)e^{ikz}$$

$$\mathrm{Re}\left[\chi(\vec{r})_{\ell=0}\right]$$



$$\chi(\vec{r})=\frac{1}{i\hbar}\int_0^\infty dt\, e^{iEt/\hbar}\psi(\vec{r},t)$$

3D lattice space calculation
Skyrme-TDDFT

Mostly the functional is local in density
→Appropriate for coordinate-space representation

Kinetic energy, current densities, etc. are estimated with the finite difference method

Skyrme TDDFT in real space

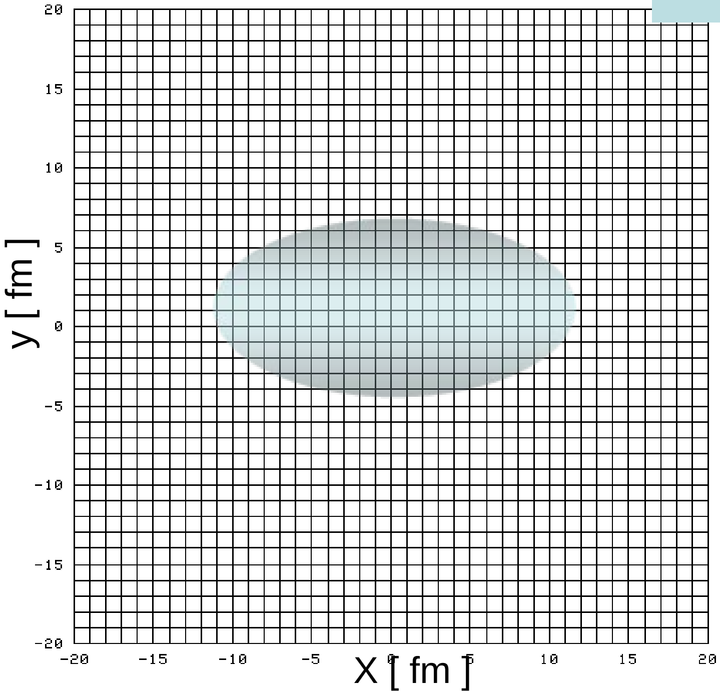
Time-dependent Kohn-Sham equation

$$- i\,\tilde{\eta}\,(r\,)$$

$$i\frac{\partial}{\partial t}\psi_i(\mathbf{r}\sigma\tau, t) = \Big(h_{\mathrm{HF}}[\rho,\tau,\mathbf{j},\mathbf{s},\overleftrightarrow{\mathbf{J}}](t) + V_{\mathrm{ext}}(t)\Big)\psi_i(\mathbf{r}\sigma\tau, t)$$

3D space is discretized in lattice

Single-particle orbital: $\varphi_i(\mathbf{r},t) = \{\varphi_i(\mathbf{r}_k, t_n)\}_{k=1,\cdots Mr}^{n=1,\cdots Mt}, \quad i = 1,\cdots,N$



N: Number of particles

Mr: Number of mesh points

Mt: Number of time slices

Spatial mesh size is about 1 fm.

Time step is about 0.2 fm/c

Nakatsukasa, Yabana, Phys. Rev. C71 (2005) 024301

Real-time calculation of response functions

1. Weak instantaneous external perturbation

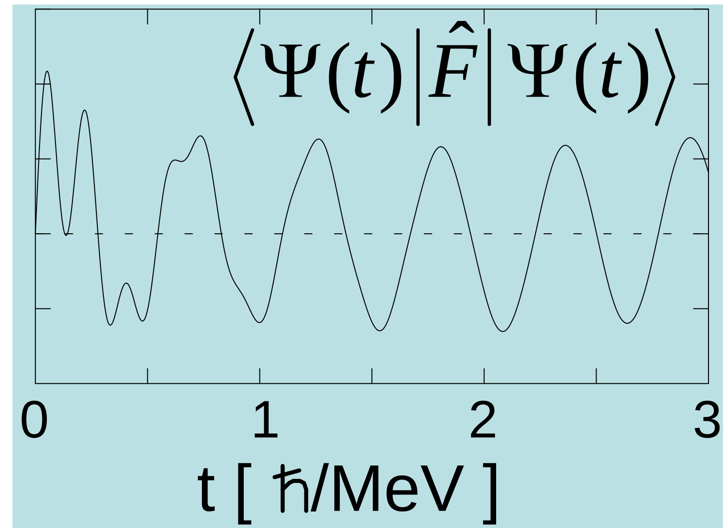
$$V_{\text{ext}}(t) = \hat{F}\delta(t)$$

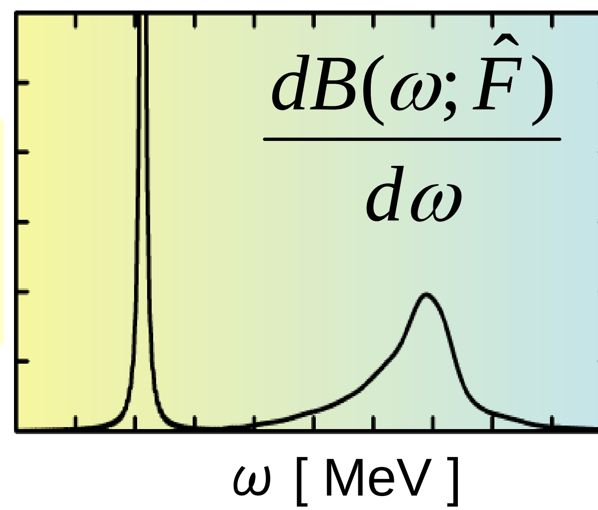
2. Calculate time evolution of

$$\left\langle \Psi(t) \middle| \hat{F} \middle| \Psi(t) \right\rangle$$

3. Fourier transform to energy domain

$$\frac{dB(\omega;\hat{F})}{d\omega} = -\frac{1}{\pi}\,\mathrm{Im}\int \left\langle \Psi(t) \middle| \hat{F} \middle| \Psi(t) \right\rangle e^{i\omega t}\,dt$$

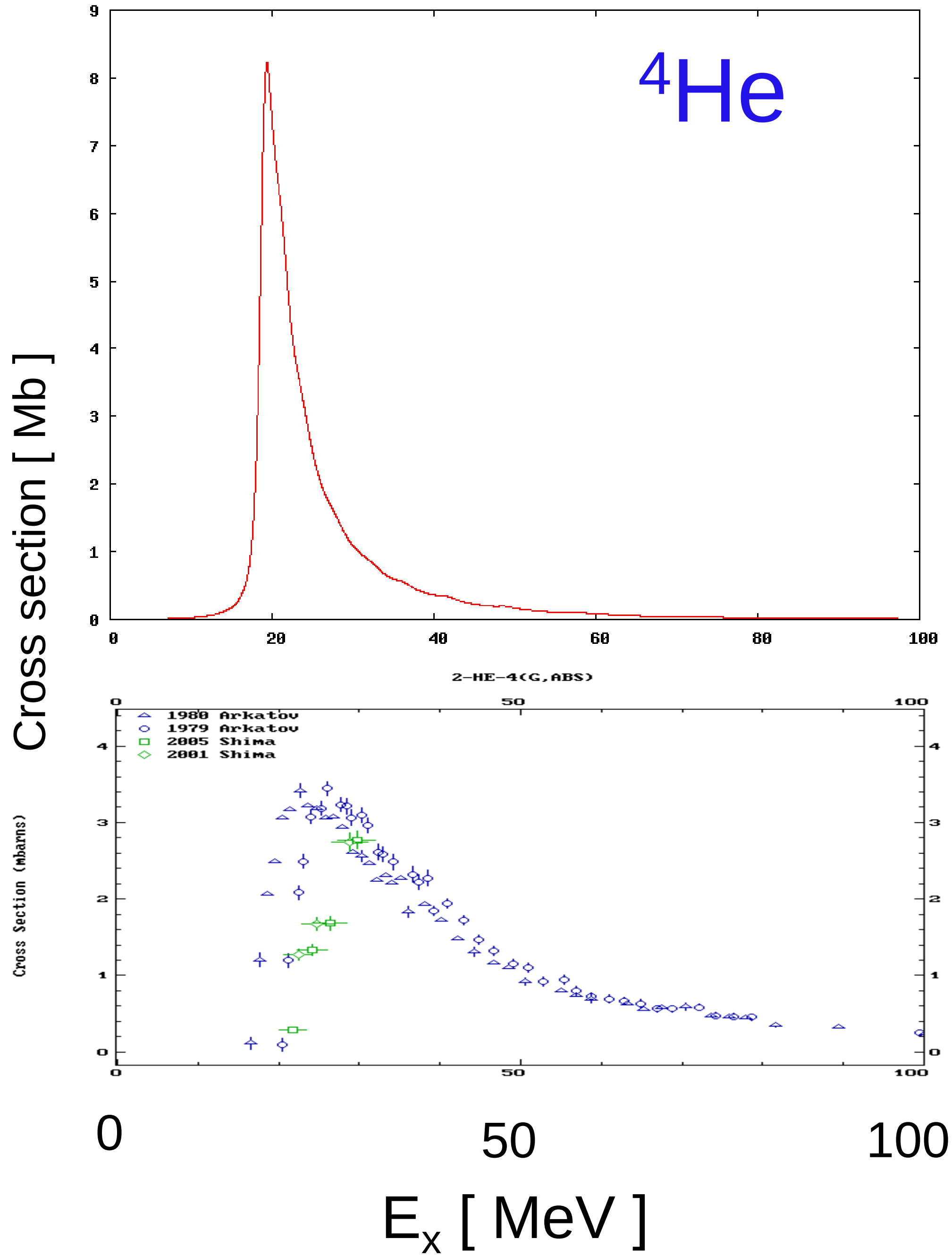


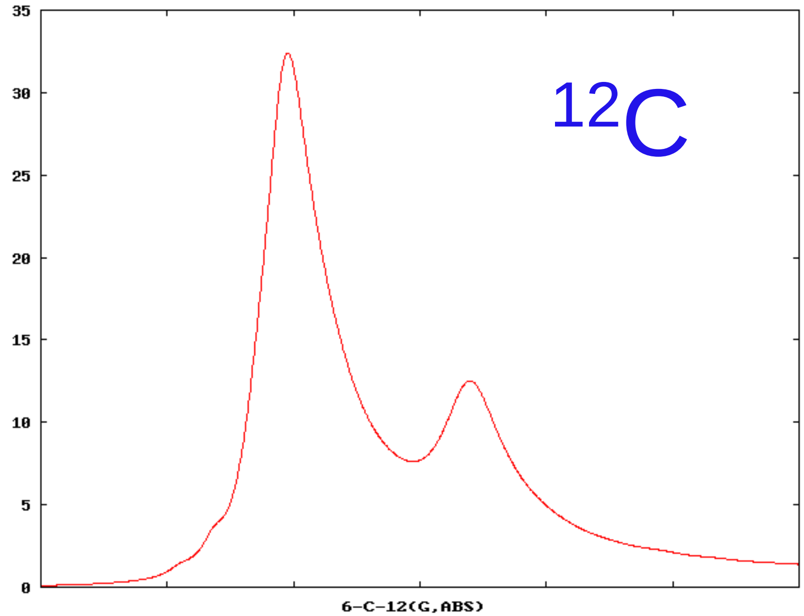


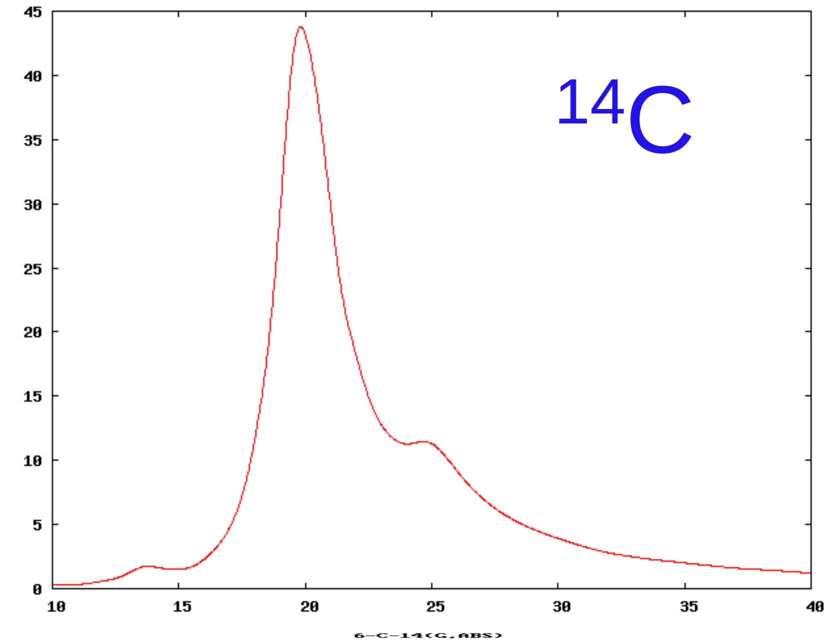
Nuclear photo-absorption cross section (IV-GDR)

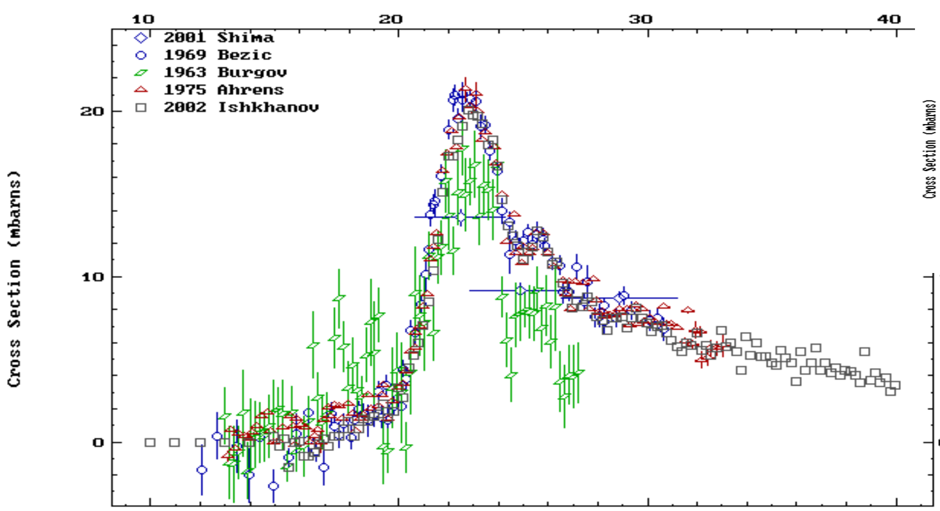
Skyrme functional with the SGII parameter set

Γ =1 MeV



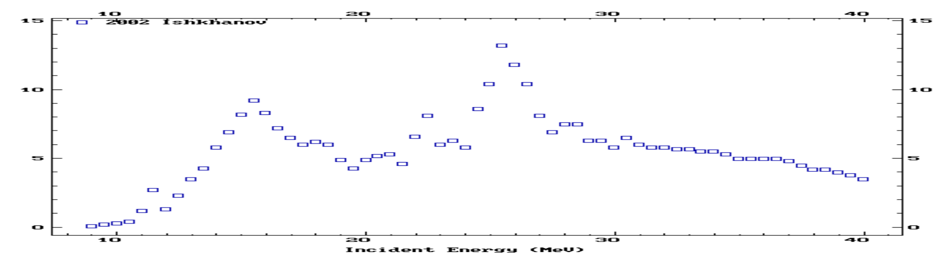






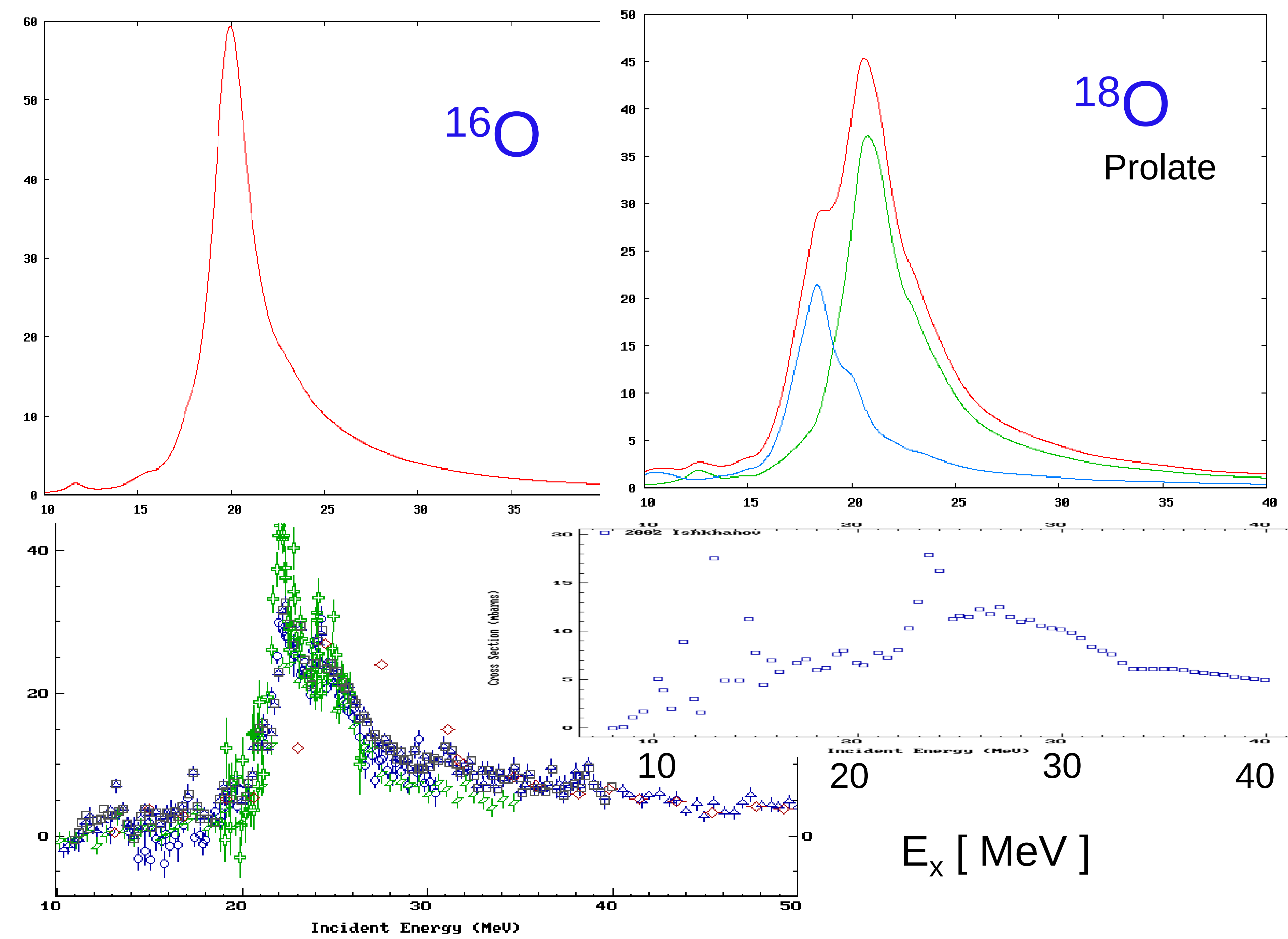
10 20 30 40

E_x [MeV]

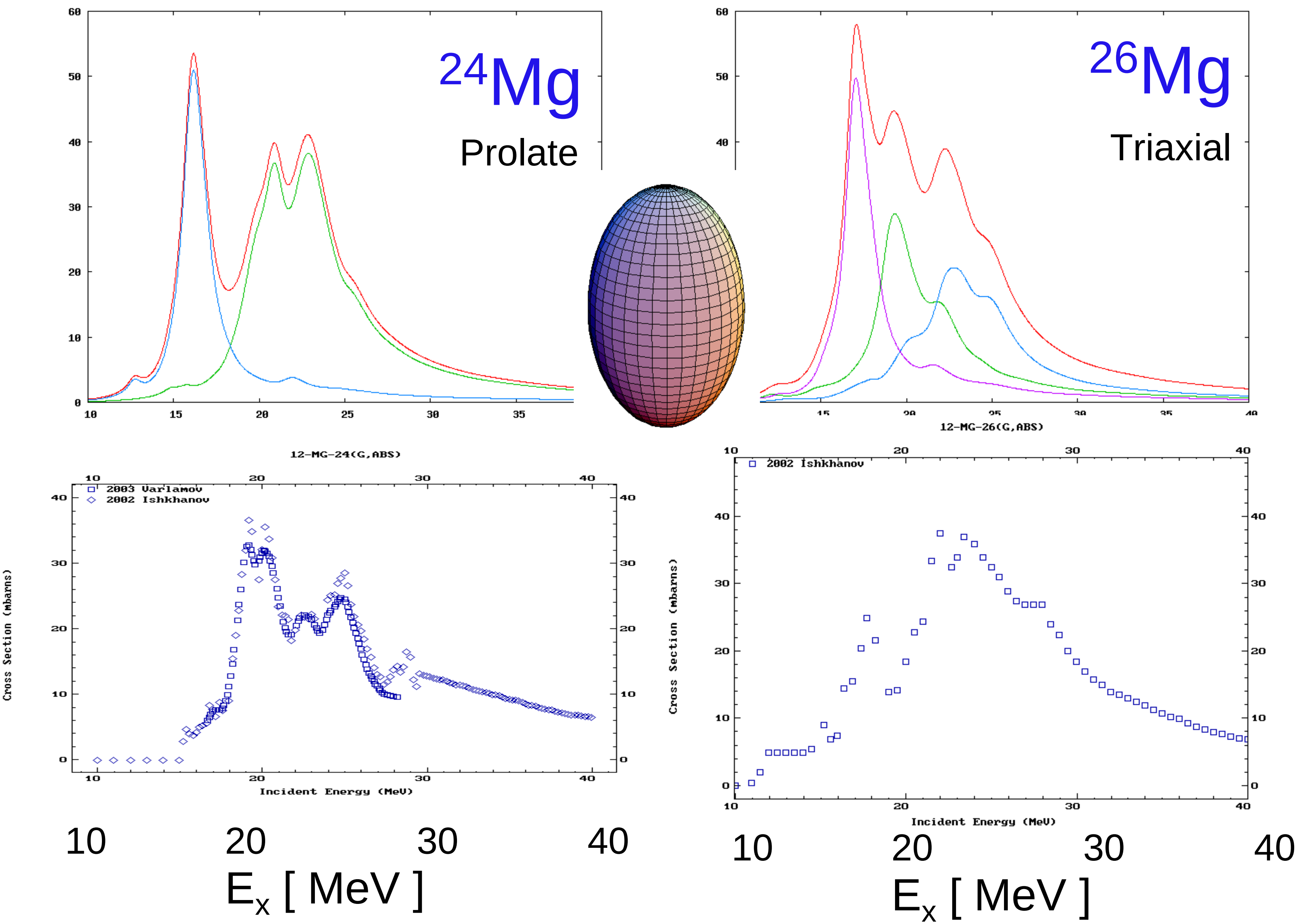


10 20 30 40

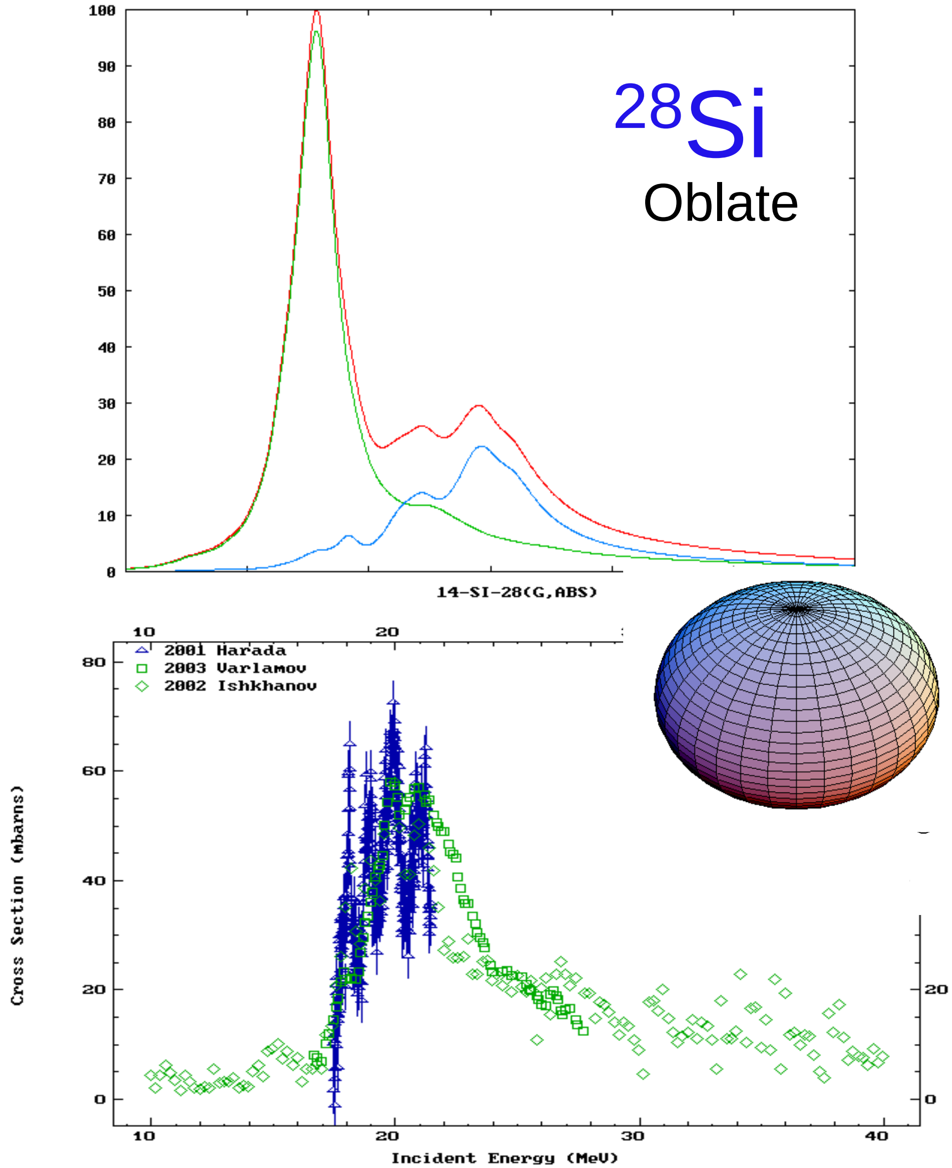
E_x [MeV]



^{16}O
^{18}O
Prolate
2002 Ishkhanov
Cross Section (mbarns)
Incident Energy (MeV)
Incident Energy (MeV)
10
20
30
40
E_x [MeV]

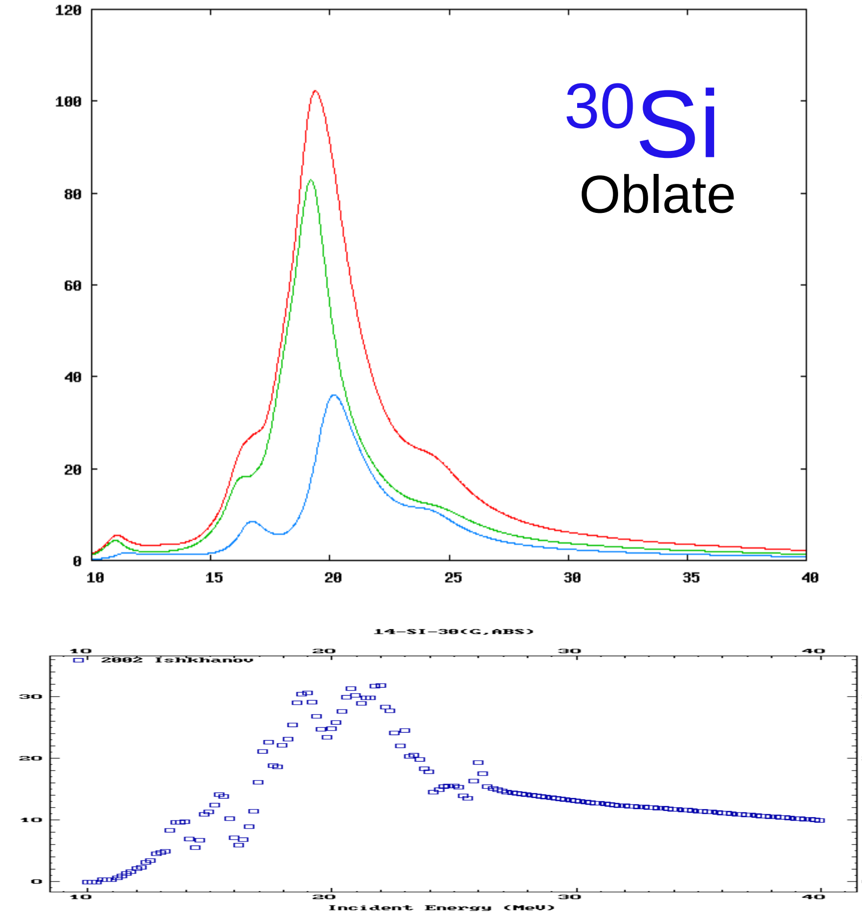


24Mg
Prolate
26Mg
Triaxial
12-MG-24(G,ABS)
12-MG-26(G,ABS)
2003 Varlamov
2002 Ishkhanov
2002 Ishkhanov
Cross Section (mbarns)
Incident Energy (MeV)
10 20 30 40
Ex [MeV]
10 20 30 40
Ex [MeV]



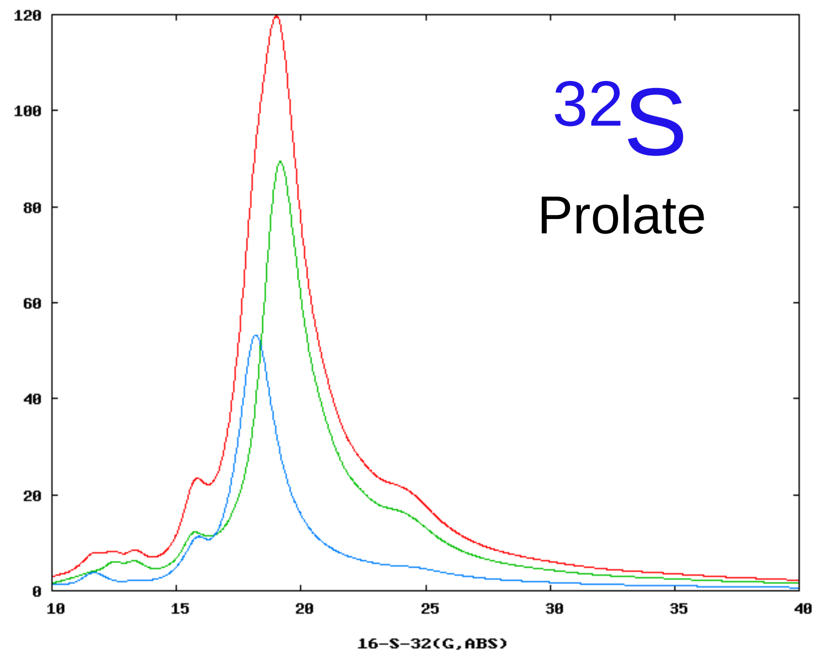
10 20 30 40

E_x [MeV]

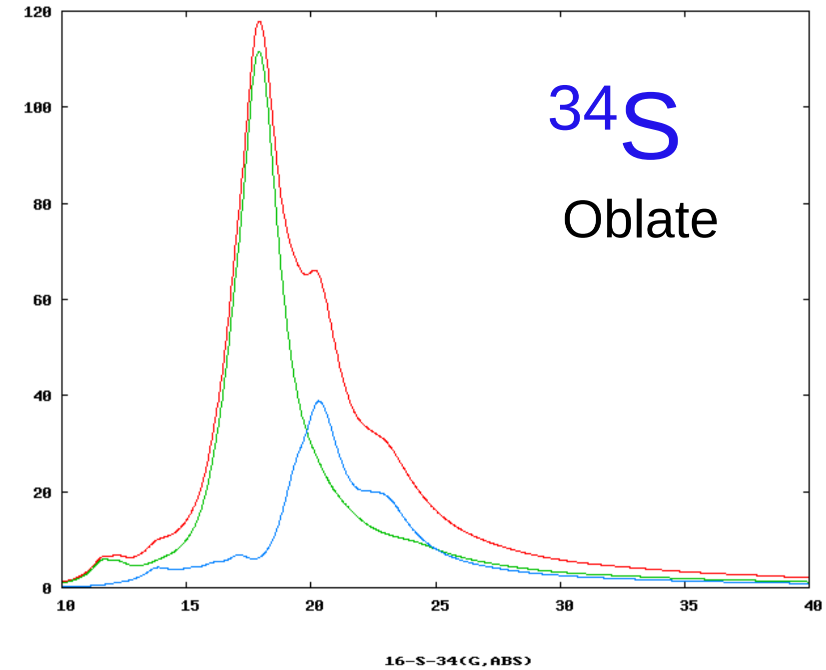


.0 20 30 40

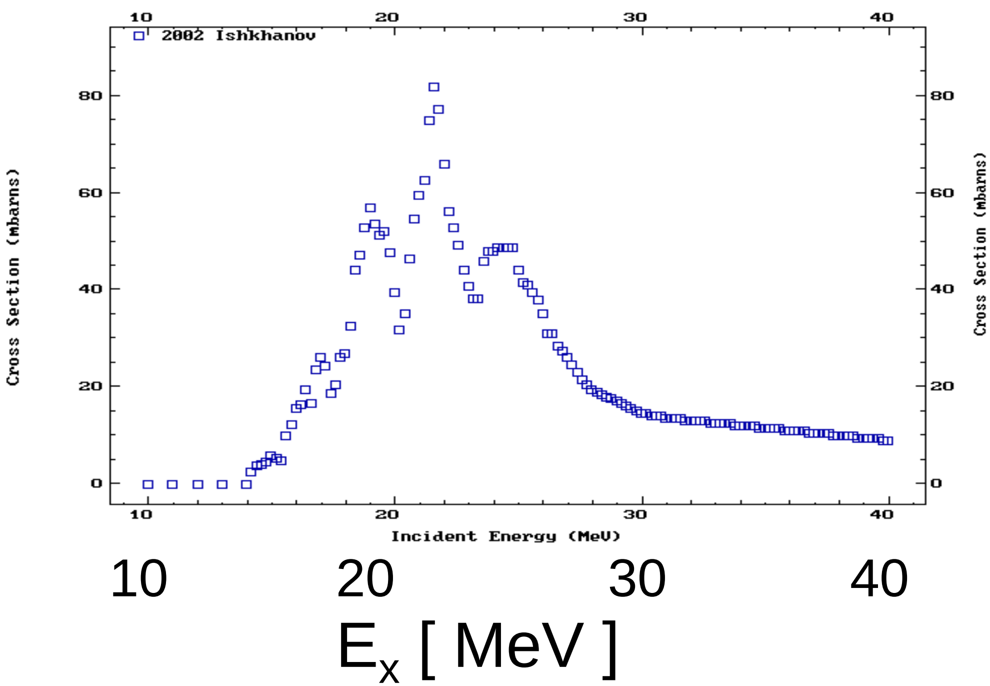
E_x [MeV]



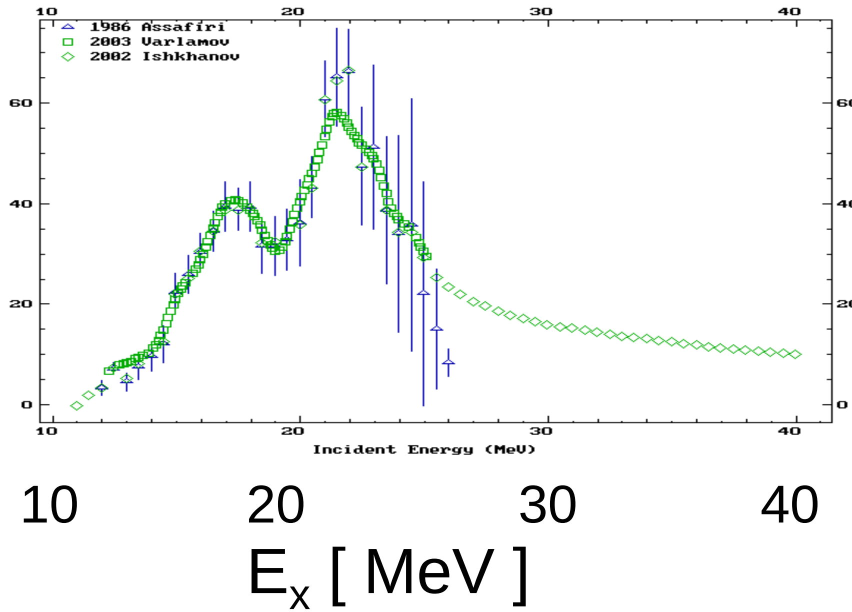
^{32}S
Prolate
16-S-32(G,ABS)



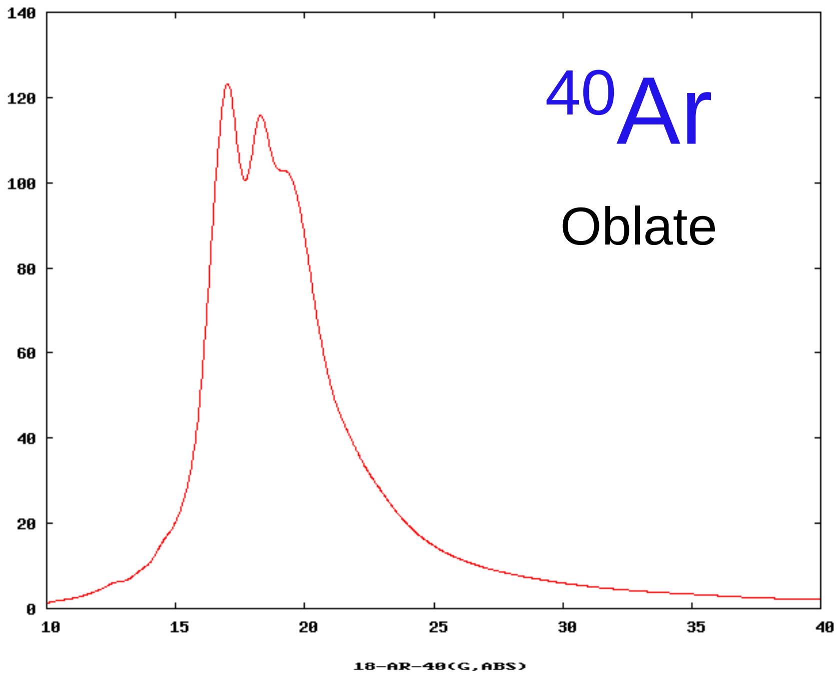
^{34}S
Oblate
16-S-34(G,ABS)

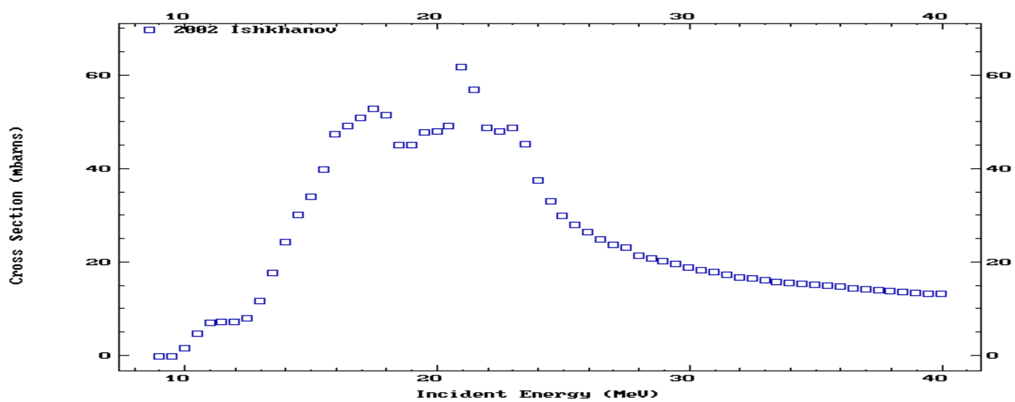


2002 Ishkhanov
Cross Section (mbarns)
Incident Energy (MeV)
10 20 30 40
E_x [MeV]



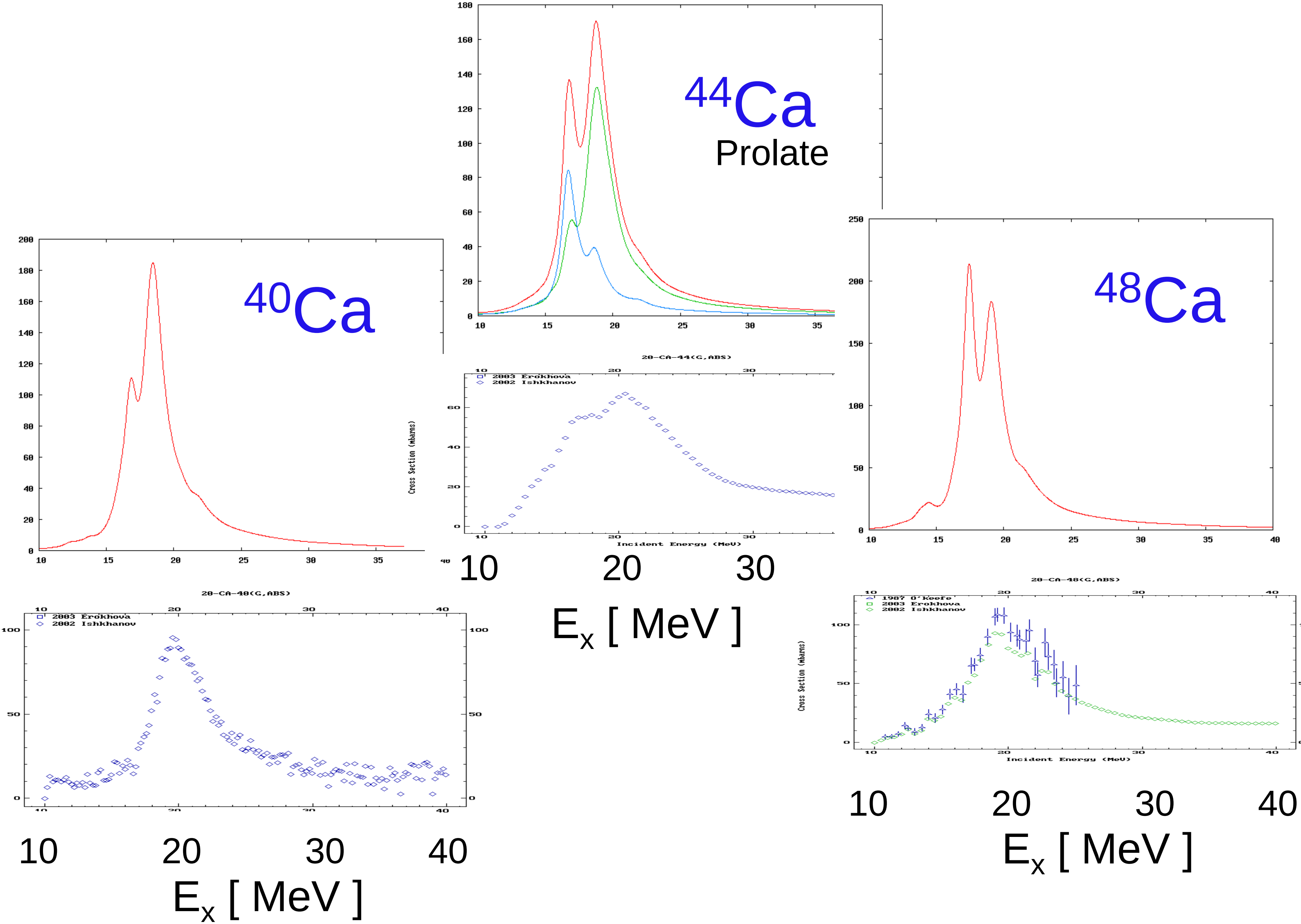
1986 Assafiri
2003 Varlamov
2002 Ishkhanov
Cross Section (mbarns)
Incident Energy (MeV)
10 20 30 40
E_x [MeV]



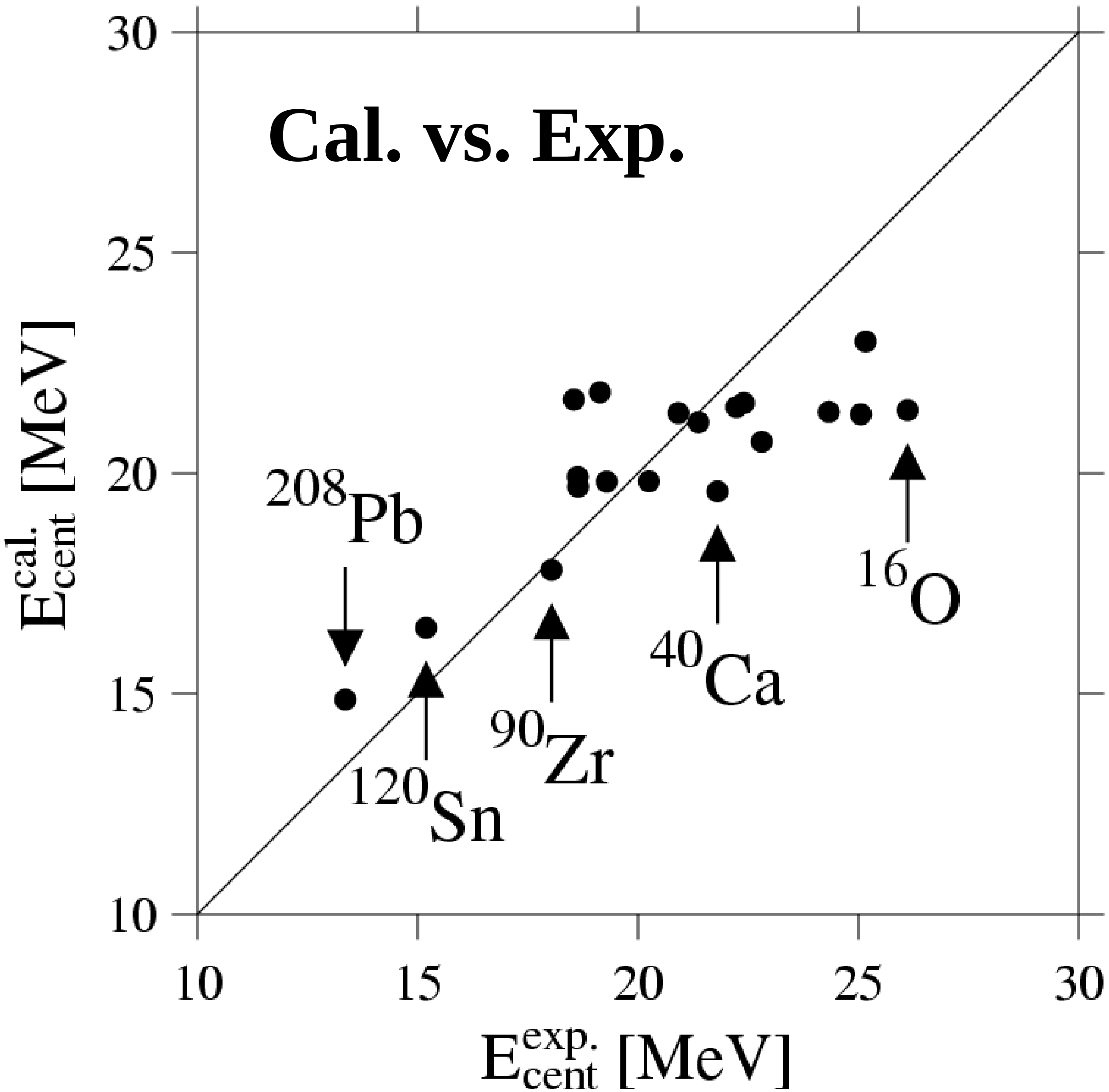


10 20 30 40

E_x [MeV]

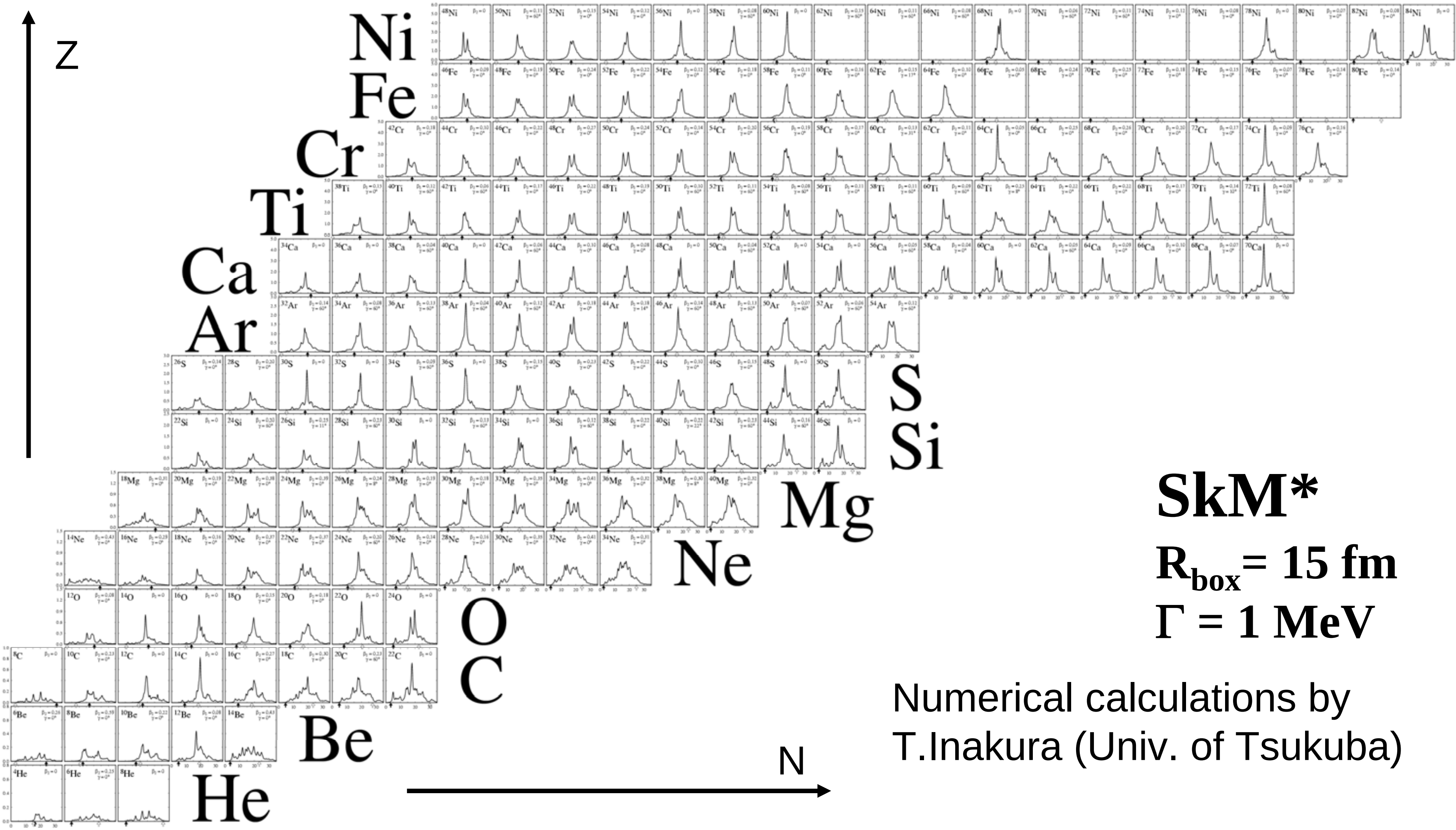


^{44}Ca
Prolate
20-CA-44(G,ABS)
2003 Erokhova
2002 Ishkhanov
Incident Energy (MeV)
10 20 30
E_x [MeV]
^{40}Ca
20-CA-40(G,ABS)
2003 Erokhova
2002 Ishkhanov
Cross Section (mbarns)
10 20 30 40
E_x [MeV]
^{48}Ca
20-CA-48(G,ABS)
1987 O'Keefe
2003 Erokhova
2002 Ishkhanov
Cross Section (mbarns)
Incident Energy (MeV)
10 20 30 40
E_x [MeV]



Cal. vs. Exp.
$E^{cal.}_{cent}$ [MeV]
$E^{exp.}_{cent}$ [MeV]
^{208}Pb
^{120}Sn
^{90}Zr
^{40}Ca
^{16}O
10
15
20
25
30

Electric dipole strengths



SkM*

R_{box}= 15 fm

Γ = 1 MeV

Numerical calculations by
T.Inakura (Univ. of Tsukuba)

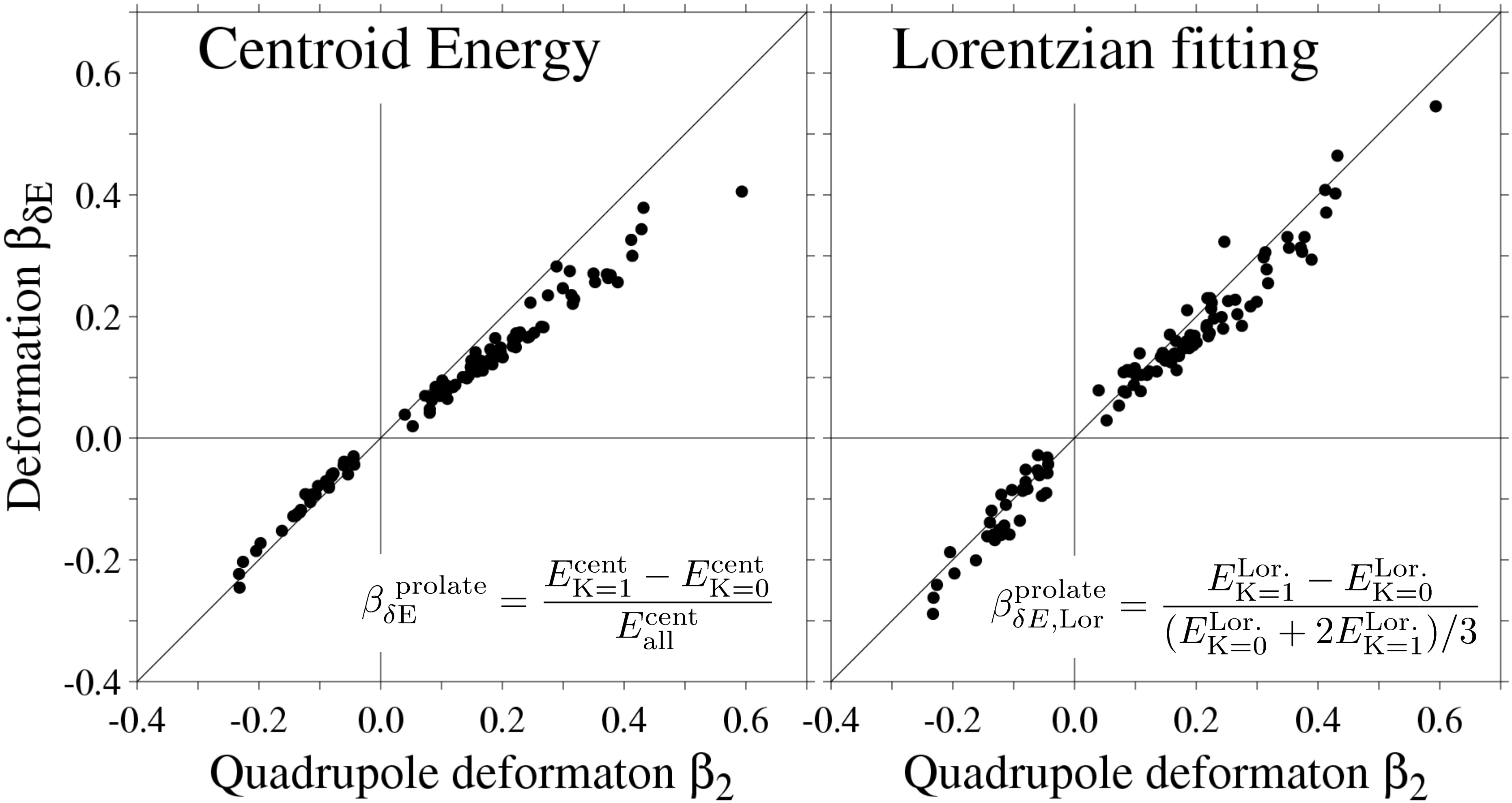
Peak splitting by deformation

3D H.O. model

$$\boxed{\beta_{\delta E} \sim \beta_2}$$

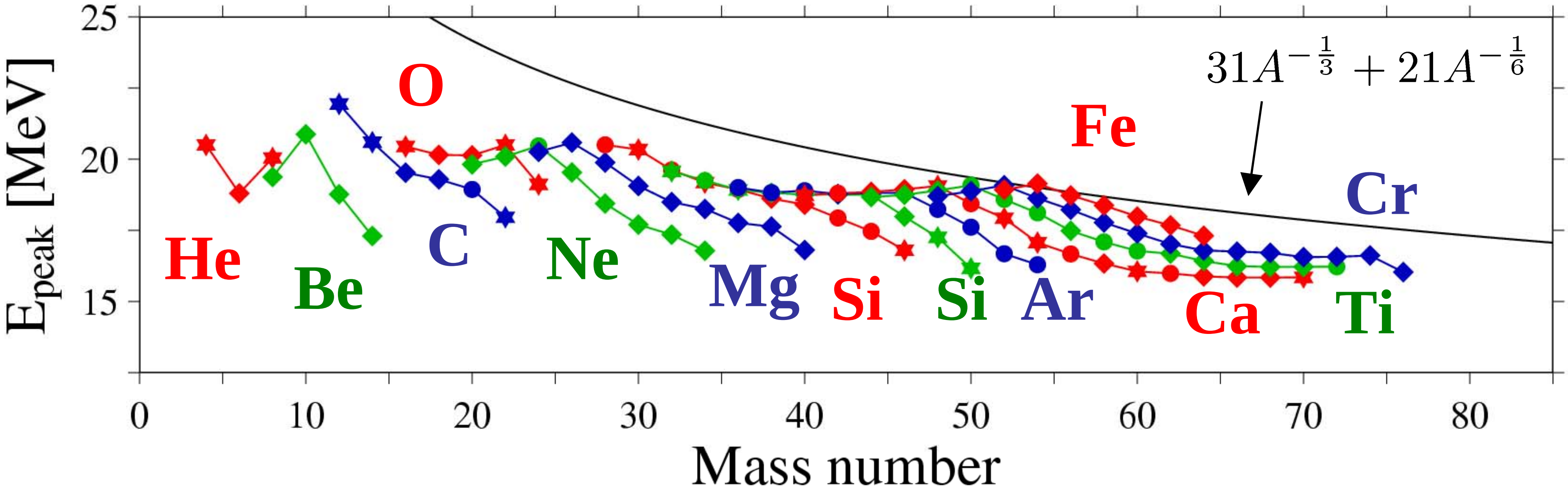
Bohr-Mottelson, text book.

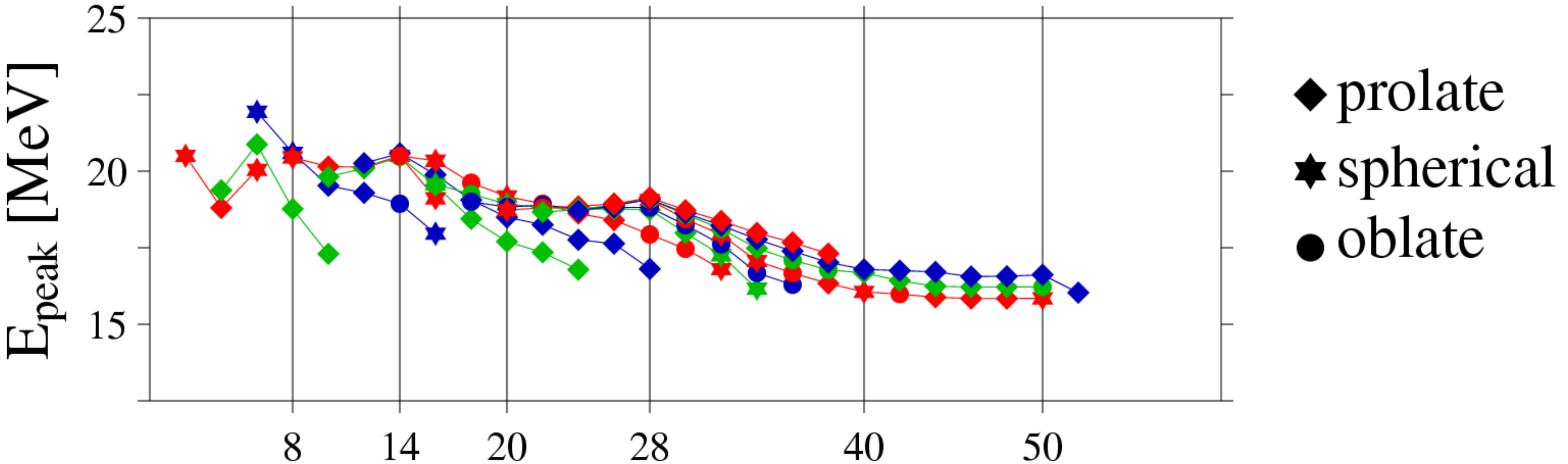
$$\beta_{2m} \;=\; \frac{4\pi}{3}\frac{\langle r^2 Y_{2m}\rangle}{\frac{5}{3}\langle r^2\rangle}$$



Centroid energy of IVGDR

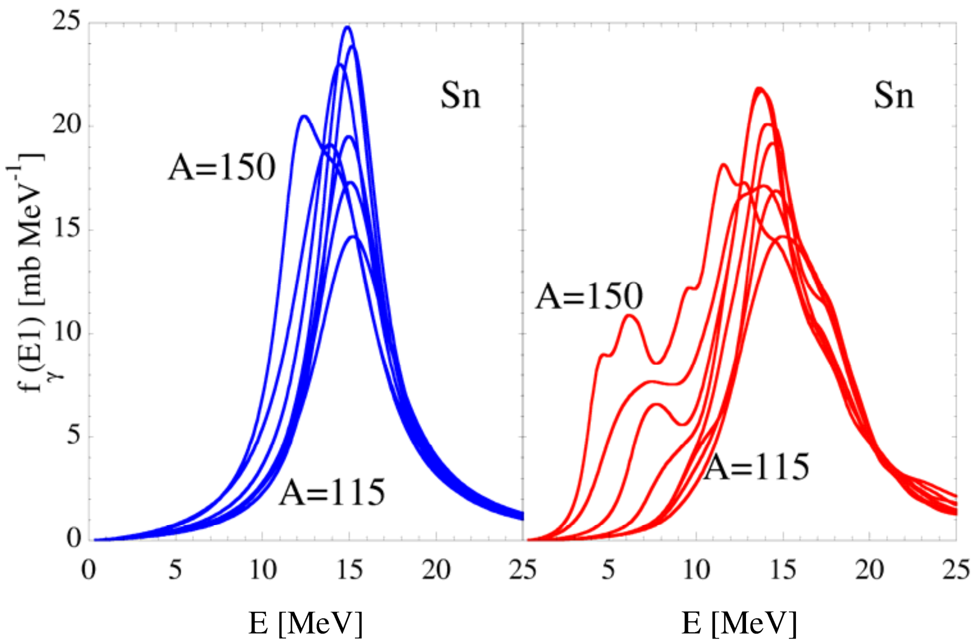
$$E_{GDR} \approx f(N,Z) \neq g(A)$$





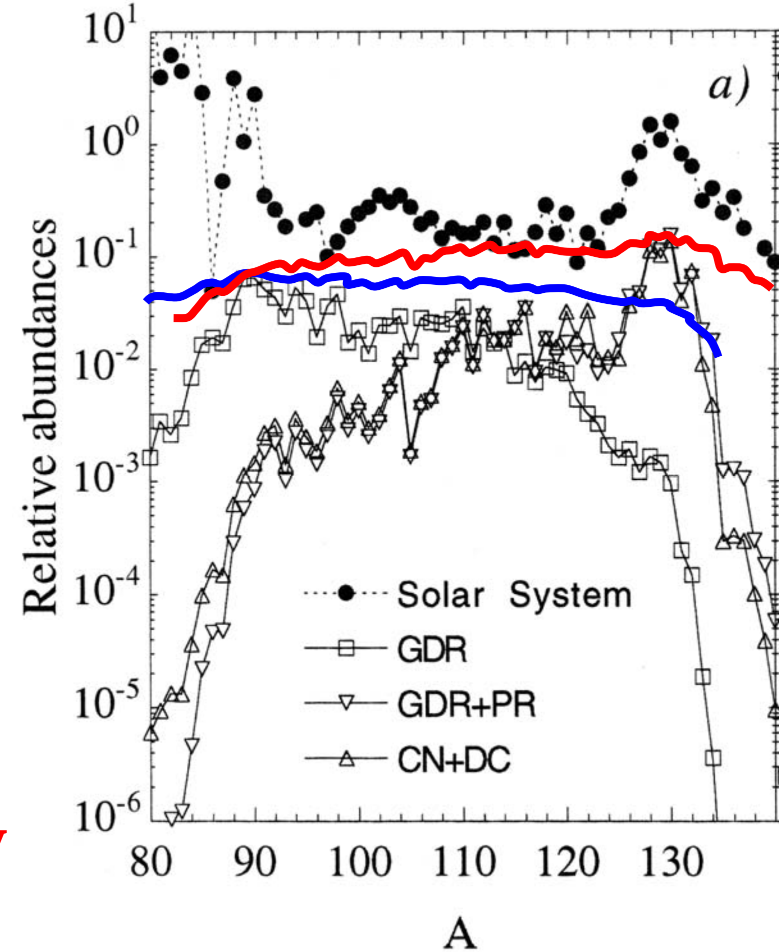
PDR: impact on the r-process

S. Goriely, Phys. Lett. **B436**, 10.

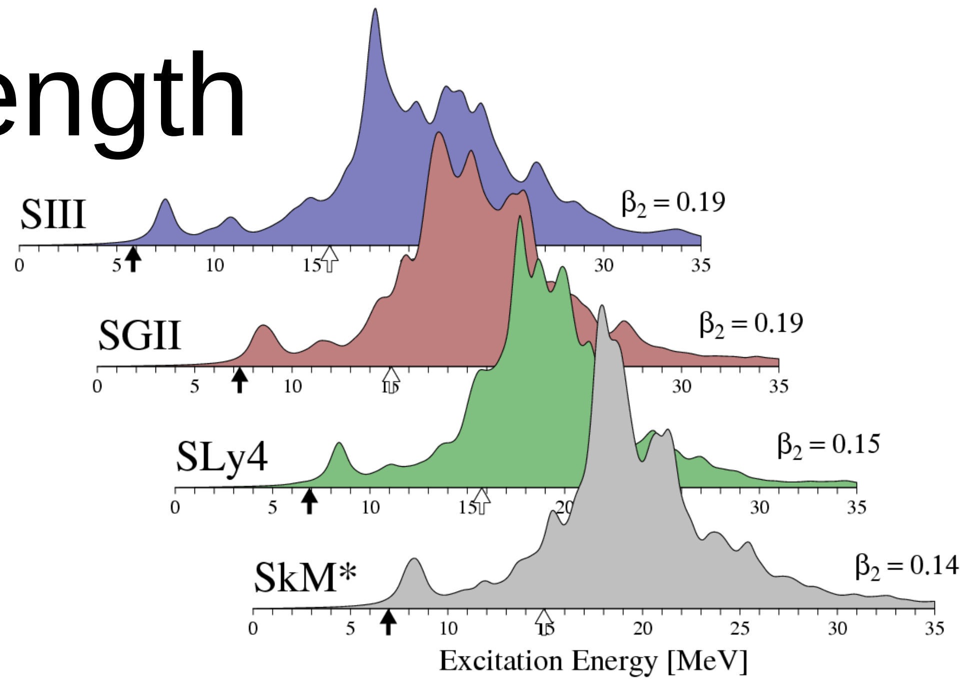


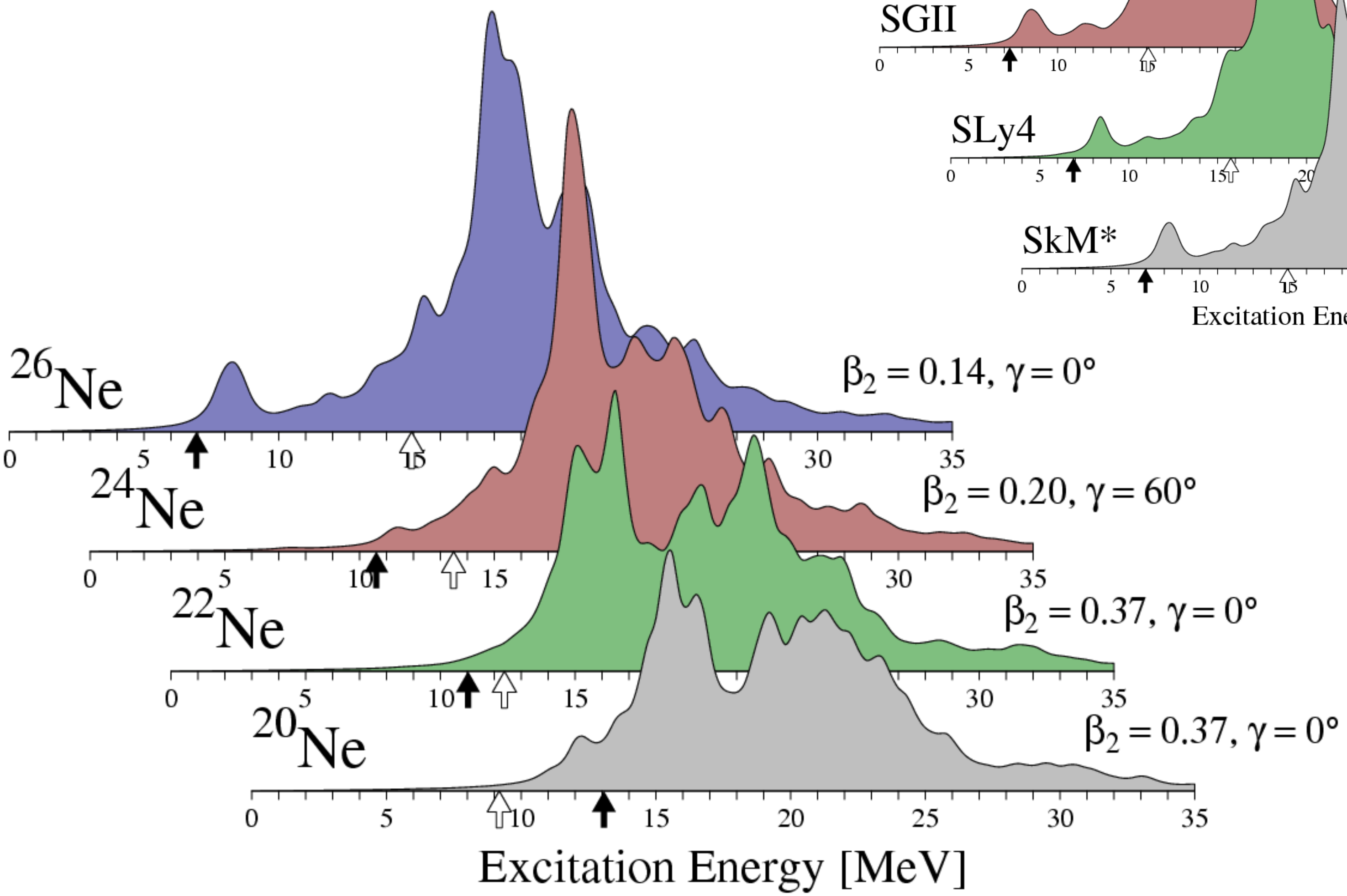
GDR
(phenom.)

GDR+pygmy
(microscopic)

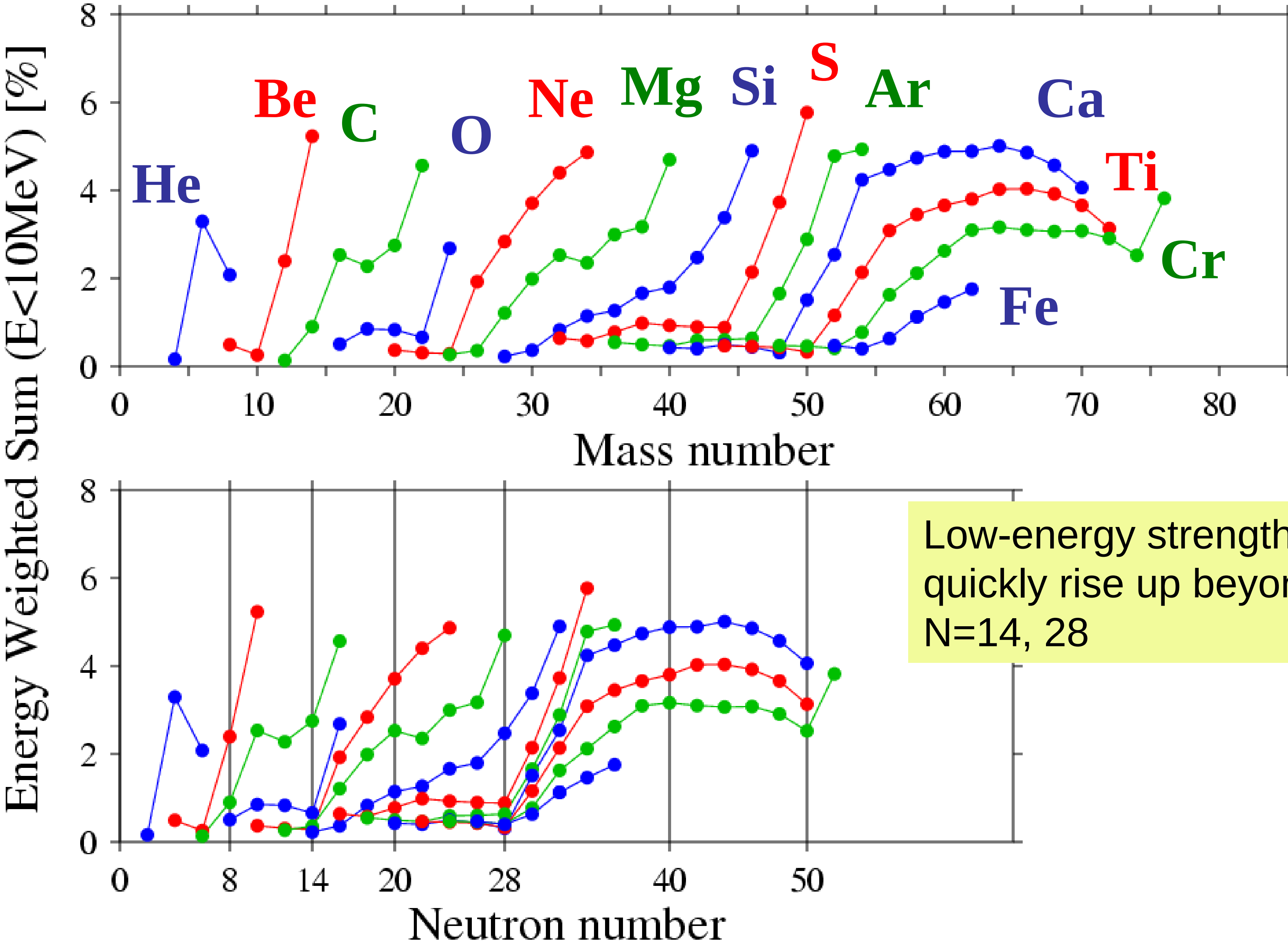


Low-energy strength





Low-lying strengths



Low-energy strengths quickly rise up beyond N=14, 28

Summary

- What DFT/TDDFT can do:
  - Systematic calculations for all nuclei including those far from the stability line
  - Nuclear matter, neutron matter, inhomogeneous nuclear matter
  - Computational Nuclear Data for photonuclear cross section
  - Description of large amplitude dynamics, such as fission